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Cincinnati Univ, OH

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This documentation contains the program listings, program flowcharts, symbols definitions, symbol references and program descriptions of all the Basic language programs which implement the functional specifications for an advanced chromatography automation system (EPA report EPA 600/4-79-038). The programs are written in Data General Extended Basic Revision 4.3.

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PROGRAM DOCUMENTATION FOR THE GAS CHROMATOGRAPHY AUTOMATION SYSTEM

by

Jonathan E. Kopke
SouthWestern Ohio Regional Computer Center
University of Cincinnati
Cincinnati, Ohio 45220

Contract No. GS-05S-10458

Project Officer

John M. Teuschler
Physical and Chemical Methods Branch
Environmental Monitoring and Support Laboratory
Cincinnati, Ohio 45268

ENVIRONMENTAL MONITORING AND SUPPORT LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
CINCINNATI, OHIO 45268

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FOREWORD

Environmental measurements are required to determine the quality of ambient waters and the character of waste effluents. The Environmental Monitoring and Support Laboratory - Cincinnati, conducts research to:

- Develop and evaluate techniques to measure the presence and concentration of physical, chemical, and radiological pollutants in water, wastewater, bottom sediments, and solid waste.
- Investigate methods for the concentration, recovery, and identification of viruses, bacteria and other microbiological organisms in water, and to determine the responses of aquatic organisms to water quality.
- Develop and operate an Agency-wide quality assurance program to assure standardization and quality control of systems for monitoring water and wastewater.
- Develop and operate a computerized system for instrument automation leading to improved data collection, analysis, and quality control.

This report was developed in the Advanced Instrumentation Section of the Environmental Monitoring and Support Laboratory in the interest of advancing laboratory techniques and quality control through computerization.

Dwight G. Ballinger
Director
Environmental Monitoring and Support
Laboratory - Cincinnati

ABSTRACT

This book contains complete documentation for the 22 programs of the EPA Gas Chromatography Automation System (GCAS). The GCAS is a system which accepts information from a commercially available chromatography data system and performs multi-point calibration, calculation of concentrations, identification of compounds, calculation of relative retention times or capacity ratios, calculation of EPA standard quality control statistics, calculation of replicate statistics, dissimilar analysis confirmation, and reporting of results to the Sample File Control System.

The programs of the GCAS are written in Data General Extended BASIC, Revision 4.3, under the operating system RDOS, Revision 6.2. In this document, there is a functional description, a functional flowchart, a symbol definition table, a program listing, and a symbol cross reference table for each of the programs. The structure of all data files is also completely described.

This report was submitted in partial fulfillment of Task No. 79-219 by the SouthWestern Ohio Regional Computer Center of the University of Cincinnati. It covers work done between January 10, 1979, and May 31, 1979, and work was completed as of May 31, 1979.

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SECTION 1

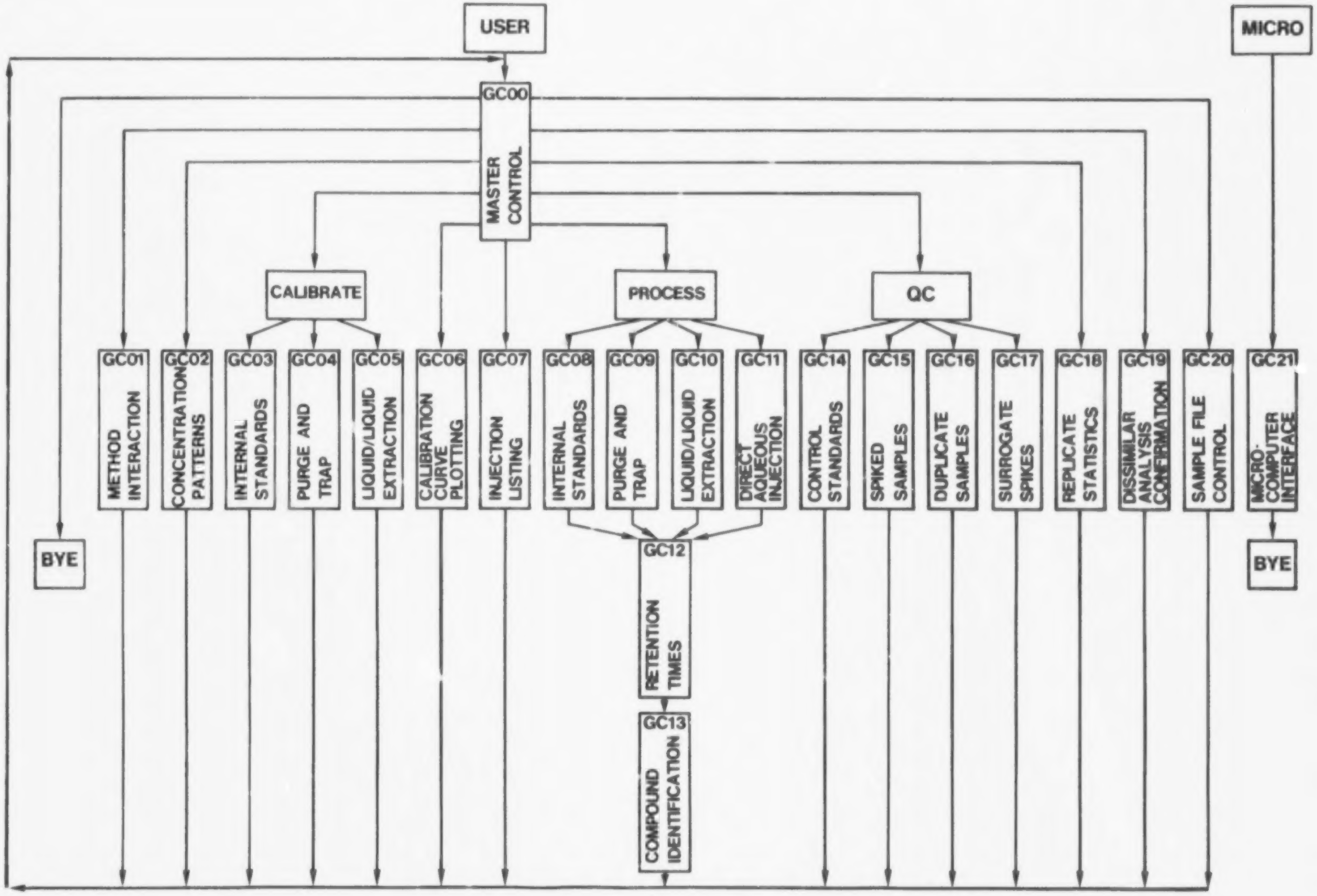
INTRODUCTION

The Gas Chromatography Automation System (GCAS) is a set of 22 computer programs which perform extensive processing of data from a commercially available chromatography data system. This book contains complete technical documentation for the programs. Two other related publications contain the functional specifications and user's guide for the GCAS.

The GCAS is written in Data General Extended BASIC, Revision 4.3, under the operating system RDOS, Revision 6.2. The 22 programs are named GC00 through GC21. The chaining relationships and functions of these programs are shown in Figure 1.

One special consideration which adds significant bulk to the GCAS is that the system handles all errors and escapes without reverting to BASIC command level. This protects the integrity of the system by not allowing any user to perform any unauthorized functions. It also makes the system easy to use by catching human errors, explaining them, and repeating the relevant questions.

The GCAS is designed to be enhanced as more advanced techniques are developed. For example, although the system accepts data only from a Varian 220L Chromatography Data System, a carefully designed replacement for program GC21 would allow the GCAS to be used with a different commercial system. Furthermore, the internal standards calibration method can be added to the GCAS by implementing programs GC03 and GC08. This document contains all information necessary for the maintenance and enhancement of the GCAC.



USER
MICRO
GC00 MASTER CONTROL
CALIBRATE
PROCESS
QC
GC01 METHOD INTERACTION
GC02 CONCENTRATION PATTERNS
GC03 INTERNAL STANDARDS
GC04 PURGE AND TRAP
GC05 LIQUID/LIQUID EXTRACTION
GC06 CALIBRATION CURVE PLOTTING
GC07 INJECTION LISTING
GC08 INTERNAL STANDARDS
GC09 PURGE AND TRAP
GC10 LIQUID/LIQUID EXTRACTION
GC11 DIRECT AQUEOUS INJECTION
GC12 RETENTION TIMES
GC13 COMPOUND IDENTIFICATION
GC14 CONTROL STANDARDS
GC15 SPIKED SAMPLES
GC16 DUPLICATE SAMPLES
GC17 SURROGATE SPIKES
GC18 REPLICATE STATISTICS
GC19 DISSIMILAR ANALYSIS CONFIRMATION
GC20 SAMPLE FILE CONTROL
GC21 MICRO-COMPUTER INTERFACE
BYE
BYE

Figure 1. Program modules and their chaining relationships.

SECTION 2

PROGRAM GC00 - MASTER CONTROL

GC00 is the master control program of the Gas Chromatography Automation System. It is entered by chaining from INITIALIZE or any of the other GC programs.

The main function of GC00 is to invoke the other programs at the option of the user. For most of the options, GC00 chains directly to the appropriate program. For calibration or processing, the program reads the type of method (internal standards, purge and trap, etc.) from the method file and then chains to the appropriate program. For quality control statistics, the program gives the user a choice of four types of quality control and then branches to the appropriate program.

GC00 also opens the method file and leaves it open when it chains to another program. Furthermore, the method file remains open when the other programs chain back to GC00. More precisely, GC00 opens the method file when it is first entered from INITIALIZE, GC01, or GC19, but not chaining to GC01 or GC19. It closes the method file when it 1) chains to GC01 or GC19, 2) chains to the Sample File Control programs RUNEDIT or SEND, or 3) logs off from the Nova.

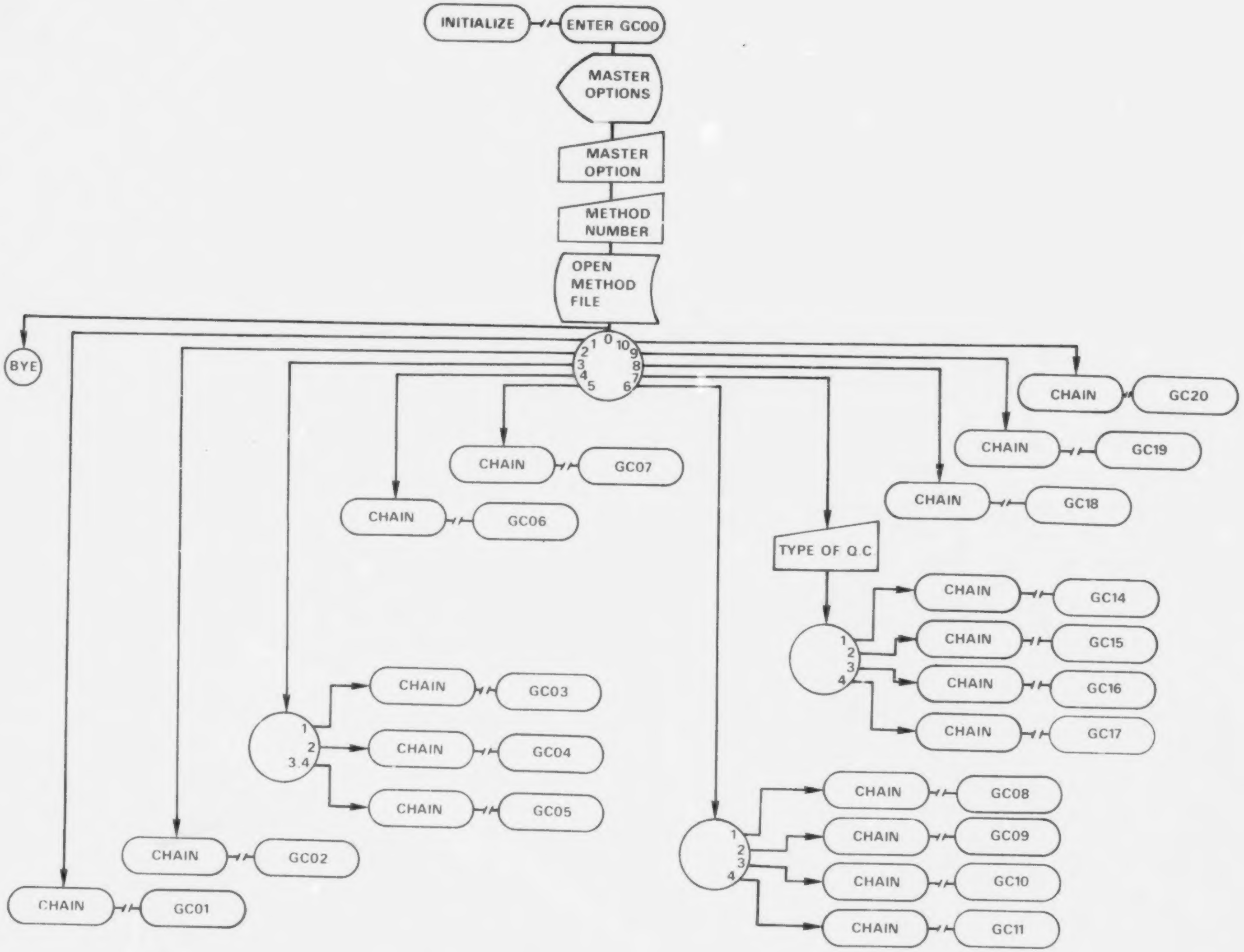

INITIALIZE
ENTER GC00
MASTER OPTIONS
MASTER OPTION
METHOD NUMBER
OPEN METHOD FILE
0
1
2
3
4
5
6
7
8
9
10
BYE
CHAIN
GC01
CHAIN
GC02
1
2
3.4
CHAIN
GC03
CHAIN
GC04
CHAIN
GC05
CHAIN
GC06
CHAIN
GC07
1
2
3
4
CHAIN
GC08
CHAIN
GC09
CHAIN
GC10
CHAIN
GC11
TYPE OF Q.C
1
2
3
4
CHAIN
GC14
CHAIN
GC15
CHAIN
GC16
CHAIN
GC17
CHAIN
GC18
CHAIN
GC19
CHAIN
GC20

Figure 2. Flowchart of Program GC00.

TABLE 1. SYMBOL DEFINITIONS FOR PROGRAM GC00

N1	the type of calibration and processing
	N1=1 internal standards N1=2 purge and trap N1=3 liquid/liquid extraction N1=4 direct aqueous injection
T	the number of the method
T$	the name of the method file
U$	the name of the user
V	a flag for keeping track of the method file
	V=0 a method file is open V=1 no method file is open
X	the user's answer to multiple choice questions
X$	the user's answer to a Y or N question

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  1
                       PROGRAM LISTING FOR GC00

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
 0030 REM   +   PROGRAM GC00, MASTER CONTROL                            +
 0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 10, 1979                +
 0050 REM   +   MOST RECENT REVISION:  APRIL 16, 1979                   +
 0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0070 REM
 0080 LET V=0
 0090 GOTO 0110
 0100 LET V=1
 0110 ON ESC THEN GOTO 0280
 0120 ESC
 0125 PAGE =74
 0126 GOTO 0280
 0130 PRINT
 0140 PRINT
 0150 PRINT "THESE ARE THE MASTER OPTIONS:"
 0160 PRINT
 0170 PRINT "     0.  SIGN OFF"
 0180 PRINT "     1.  METHOD INTERACTION"
 0190 PRINT "     2.  CONCENTRATION PATTERN INTERACTION"
 0200 PRINT "     3.  CALIBRATION"
 0210 PRINT "     4.  CALIBRATION CURVE PLOTTING"
 0220 PRINT "     5.  INJECTION LISTING"
 0230 PRINT "     6.  PROCESSING"
 0240 PRINT "     7.  QUALITY CONTROL"
 0250 PRINT "     8.  REPLICATE STATISTICS"
 0260 PRINT "     9.  DISSIMILAR ANALYSIS CONFIRMATION"
 0270 PRINT "    10.  SAMPLE FILE CONTROL"
 0275 GOTO 0285
 0280 PRINT
 0285 PRINT
 0290 TIME =120
 0300 ON ERR THEN GOTO 0340
 0310 TINPUT "WHICH MASTER OPTION DO YOU WANT TO USE?  (0-10, OR 'RETUR
*     N' FOR HELP)  ",X$
 0320 ON ERR THEN STOP
 0325 IF LEN(X$)=0 THEN GOTO 0140
 0326 ON ERR THEN GOTO 0405
 0327 LET X=VAL(X$)
 0328 ON ERR THEN STOP
 0330 GOTO 0360

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  2
                       PROGRAM LISTING FOR GC00

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0340 ON ERR THEN STOP
 0350 IF SYS(7)=60 THEN GOTO 0370
 0360 IF X<>0 THEN GOTO 0400
 0370 PRINT
 0380 PRINT "YOU ARE BEING SIGNED OFF FROM THE NOVA BY THIS PROGAM."
 0385 CLOSE
 0390 BYE
 0400 IF X=INT(X) THEN IF X>0 THEN IF X<11 THEN GOTO 0460
 0405 ON ERR THEN STOP
 0410 PRINT
 0420 PRINT "<7><7>";X$;" IS NOT A VALID OPTION NUMBER."
 0430 GOTO 0140
 0440 REM   -----------------------------------------------------------
 0450 REM          OPEN THE METHOD FILE
 0460 IF V<>1 THEN GOTO 0770
 0470 IF X=1 THEN GOTO 0770
 0480 IF X=9 THEN GOTO 0770
 0490 PRINT
 0500 ON ERR THEN GOTO 0520
 0510 INPUT "WHAT IS THE NUMBER OF THE METHOD YOU WANT TO USE?  ",T
 0520 ON ERR THEN STOP
 0530 IF T=ABS(INT(T)) THEN IF T<=9999 THEN GOTO 0570
 0540 PRINT
 0550 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
 0560 GOTO 0490
 0570 LET T$="GC0000"
 0580 LET T$[7-LEN(STR$(T)),6]=STR$(T)
 0590 ON ERR THEN GOTO 0610
 0600 RENAME T$,T$
 0610 ON ERR THEN STOP
 0620 IF SYS(7)<>-48 THEN GOTO 0650
 0630 DELAY =1
 0640 GOTO 0590
 0650 IF SYS(7)=-9 THEN GOTO 0690
 0660 PRINT
 0670 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*     ];"."
 0680 GOTO 0490
 0690 ON ERR THEN GOTO 0730
 0700 OPEN FILE[4,0],T$,200
 0710 ON ERR THEN STOP
 0720 GOTO 0770

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  3
                       PROGRAM LISTING FOR GC00

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0730 ON ERR THEN STOP
0740 DELAY =1
0750 GOTO 0690
0770 ON X THEN GOTO 0800, 0850, 0890, 0960, 1000, 1040, 1120, 1350, 13
*    90, 1440
0780 REM  ----------------------------------------------------------
0790 REM          INTERACT WITH METHOD
0800 CLOSE
0810 NOESC
0820 CHAIN "GC01"
0830 REM  ----------------------------------------------------------
0840 REM          INTERACT WITH CONCENTRATION PATTERNS
0850 NOESC
0860 CHAIN "GC02"
0870 REM  ----------------------------------------------------------
0880 REM          CALIBRATE
0890 NOESC
0895 READ FILE[4,1],T$,U$,N1
0900 ON N1 THEN GOTO 0910, 0920, 0930, 0930
0910 CHAIN "GC03"
0920 CHAIN "GC04"
0930 CHAIN "GC05"
0940 REM  ----------------------------------------------------------
0950 REM          EXAMINE CALIBRATION CURVES
0960 NOESC
0970 CHAIN "GC06"
0980 REM  ----------------------------------------------------------
0990 REM          LIST EXTANT INJECTIONS
1000 NOESC
1010 CHAIN "GC07"
1020 REM  ----------------------------------------------------------
1030 REM          PROCESS INJECTIONS
1040 NOESC
1045 READ FILE[4,1],T$,U$,N1
1050 ON N1 THEN GOTO 1060, 1070, 1080, 1090
1060 CHAIN "GC08"
1070 CHAIN "GC09"
1080 CHAIN "GC10"
1090 CHAIN "GC11"
1100 REM  ----------------------------------------------------------
1110 REM          CALCULATE QUALITY CONTROL STATISTICS
1120 PRINT

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  4
                       PROGRAM LISTING FOR GC00

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1130 PRINT "THESE ARE THE TYPES OF QUALITY CONTROL STATISTICS:"
1140 PRINT
1150 PRINT "    1.  CONTROL (CHECK) STANDARDS"
1160 PRINT "    2.  SPIKED SAMPLES"
1170 PRINT "    3.  DUPLICATE SAMPLES"
1180 PRINT "    4.  SURROGATE SPIKES"
1190 PRINT
1200 ON ERR THEN GOTO 1220
1210 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
1220 ON ERR THEN STOP
1230 IF X=INT(X) THEN IF X>0 THEN IF X<5 THEN GOTO 1270
1240 PRINT
1250 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
1260 GOTO 1120
1270 NOESC
1280 ON X THEN GOTO 1290, 1300, 1310, 1320
1290 CHAIN "GC14"
1300 CHAIN "GC15"
1310 CHAIN "GC16"
1320 CHAIN "GC17"
1330 REM  ----------------------------------------------------------
1340 REM          CALCULATE REPLICATE STATISTICS
1350 NOESC
1360 CHAIN "GC18"
1370 REM  ----------------------------------------------------------
1380 REM          PERFORM DISSIMILAR ANALYSIS CONFIRMATION
1390 CLOSE
1400 NOESC
1410 CHAIN "GC19"
1420 REM  ----------------------------------------------------------
1430 REM          REPORT RESULTS TO SAMPLE FILE CONTROL
1440 NOESC
1450 CHAIN "GC20"

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  5
                         SYMBOL TABLE FOR GC00

SYMBOL   REFERENCES
------  ----------------------------------------------------------------
 0110   0090
 0140   0325  0430
 0280   0110  0126
 0285   0275
 0340   0300
 0360   0330
 0370   0350
 0400   0360
 0405   0326
 0460   0400
 0490   0560  0680
 0520   0500
 0570   0530
 0590   0640
 0610   0590
 0650   0620
 0690   0650  0750
 0730   0690
 0770   0460  0470  0480  0720
 0800   0770
 0850   0770
 0890   0770
 0910   0900
 0920   0900
 0930   0900
 0960   0770
 1000   0770
 1040   0770
 1060   1050
 1070   1050
 1080   1050
 1090   1050
 1120   0770  1260
 1220   1200
 1270   1230
 1290   1280
 1300   1280
 1310   1280
 1320   1280
 1350   0770
 1390   0770
 1440   0770
 FL#4   0700  0895  1045
 N1     0895  0900  1045  1050
 T      0510  0530  0550  0580
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  6
                         SYMBOL TABLE FOR GC00

SYMBOL   REFERENCES
------  ----------------------------------------------------------------
 T$     0570  0580  0600  0670  0700  0895  1045
 U$     0895  1045
 V      0080  0100  0460
 X      0327  0360  0400  0470  0480  0770  1210  1230  1250  1280
 X$     0310  0325  0327  0420
```

SECTION 3

PROGRAM GC01 - METHOD INTERACTION

GC01 is the program which generates, modifies, deletes, and displays GCAS method files. This program is entered by chaining from GC00 (the master control program), and it chains back to that program if the escape key is pressed.

As GC01 begins, it displays the four types of method interactions which are possible, inputs the user's choice, and then branches to the appropriate section of code.

GENERATE A NEW METHOD

To generate a new method, GC01 first inputs the method number. If the specified method number is not a positive integer of four or fewer digits, a message is printed telling the user that the method number is invalid. The program then creates the name of the method file and attempts to rename that file with its own name. This step always causes an error which is trapped. If the error number is -9, there is already a method file in existence with the specified number. The user is informed of this fact, and the program branches back to the original four choices.

If the specified method number is usable, the program inputs the name of the user, the type of calibration and processing, the type of retention time calculations, and either the relative retention time reference identifier or the dead volume time. These items are written into the first record of the method file. The program then inputs the identifiers, the true names of compounds, and CAS Registry numbers for the method and writes these into the method file. When the user types the word "END" as an identifier, the program closes the method file and asks if the method should be displayed. If the user wants to have the method displayed, the program branches to that routine. Otherwise, it chains back to GC00.

MODIFY AN EXISTING METHOD

If a user wants to modify a method, this program asks for the method number. It checks whether the method number is reasonable and whether the method file already exists, as described above. It then presents four types of modifications, inputs the user's choice, and branches to the appropriate section of code.

Add Another Identifier

If the user wants to modify the method by adding another identifier, the program simply locates the end of the method file and then branches to the section for generating a new method. That section then appends additional identifiers to the method file. All of the concentration pattern files for the method are deleted.

Delete an Identifier

If the user wants to delete an identifier, the program inputs the identifier and searches through the method file for it. If the specified identifier is not in the method file, a message to that effect is printed. If the specified identifier is found in the method file, it is replaced by the dummy entry "99999." After either circumstance, the program asks whether the user wants to deal further with any method, and then either branches back to the original four choices in this program or chains back to GC00.

Add Another Compound to an Identifier

If the user wants to add another compound to the list of those associated with an identifier, this program first inputs the identifier and searches for it in the method file. If there is no matching identifier in the method file, or if the specified identifier already has the limit of three compounds associated with it, an appropriate message is printed. Otherwise, the additional compound name and CAS number are input and written into the method file. Then the program asks whether the user wants to deal further with any method, and it branches accordingly.

Change Retention Time Data

If the user wants to change retention time data, this section of code provides the choice of relative retention time or capacity ratio calculations. If the user selects relative retention time, the program asks for the identifier of the compound to whose retention time all others are relative. If the user selects capacity ratio, the program asks for the dead volume time. In either case, the data items are written into the method file.

DELETE AN EXISTING METHOD

If the user wants to delete an existing method, this program inputs the method number and checks whether the number is reasonable and whether the corresponding method file actually exists. If the file does exist, it is deleted and that event is confirmed to the user. Also, all of the concentration pattern files for the method are deleted. The program then asks if the user wants to deal further with any method and branches accordingly.

DISPLAY AN EXISTING METHOD

If the user wants to display an existing method, this program again inputs the method number and checks whether the corresponding method file actually exists. It then prints headings and the compound identification information from the method file. The program then asks if the user wants to deal further with any method and branches accordingly.

SUBROUTINE TO CHECK CAS NUMBERS

Whenever a user enters a CAS Registry number, GC01 branches to this subroutine to check whether the number is reasonable. A carriage return alone is always accepted as a valid CAS number. The subroutine does not check whether the CAS number is the correct number for the compound named; it only checks the form of the number.

CAS Registry numbers are always of the form

$$d_8d_7d_6d_5d_4d_3\text{-}d_2d_1\text{-}d_0$$

where d_n is a numeric digit. Any of the digits d_4 through d_8 may be blanks, although no embedded blanks are allowed. The positions of the hyphens never vary. Digit d_0 is a check digit which is used to verify that the number has been typed correctly. The check digit is the remainder from the following division:

$$\frac{\sum_{i=1}^{8} i\cdot(d_i)}{10}$$

In this subroutine, the CAS number typed by the user is first padded on the left with spaces until it is 11 characters long. Then if the seventh and tenth characters are not hyphens, the number is immediately identified as invalid. If the hyphens are in the correct positions, the subroutine begins the calculation for the check digit. In doing this, the subroutine must convert each digit from a string to a number. If there is any non-numeric character in the CAS number, an error results, and the number is invalid. Finally, if the calculated check digit does not match the input check digit, the CAS number is invalid. Valid CAS numbers are returned to the invoking procedure changed only by having been padded with blanks. Invalid CAS numbers are changed to "99999" before being returned to the invoking procedure. If the main program finds that a returning CAS number is "99999," it prints an error message and asks for another CAS number.

SUBROUTINE TO CHANGE SLASHES TO COMMAS

The names of many chemical compounds have commas in them, but BASIC does not allow commas to be part of an answer to an INPUT statement. Therefore, this program is set up to allow the user to type a slash where a commas is needed in an identifier or in the name of a compound, and this subroutine substitutes a comma for every slash.

SUBROUTINE TO DELETE CONCENTRATION PATTERNS

This subroutine simply loops through the 26 possible concentration pattern file names, and deletes them all.

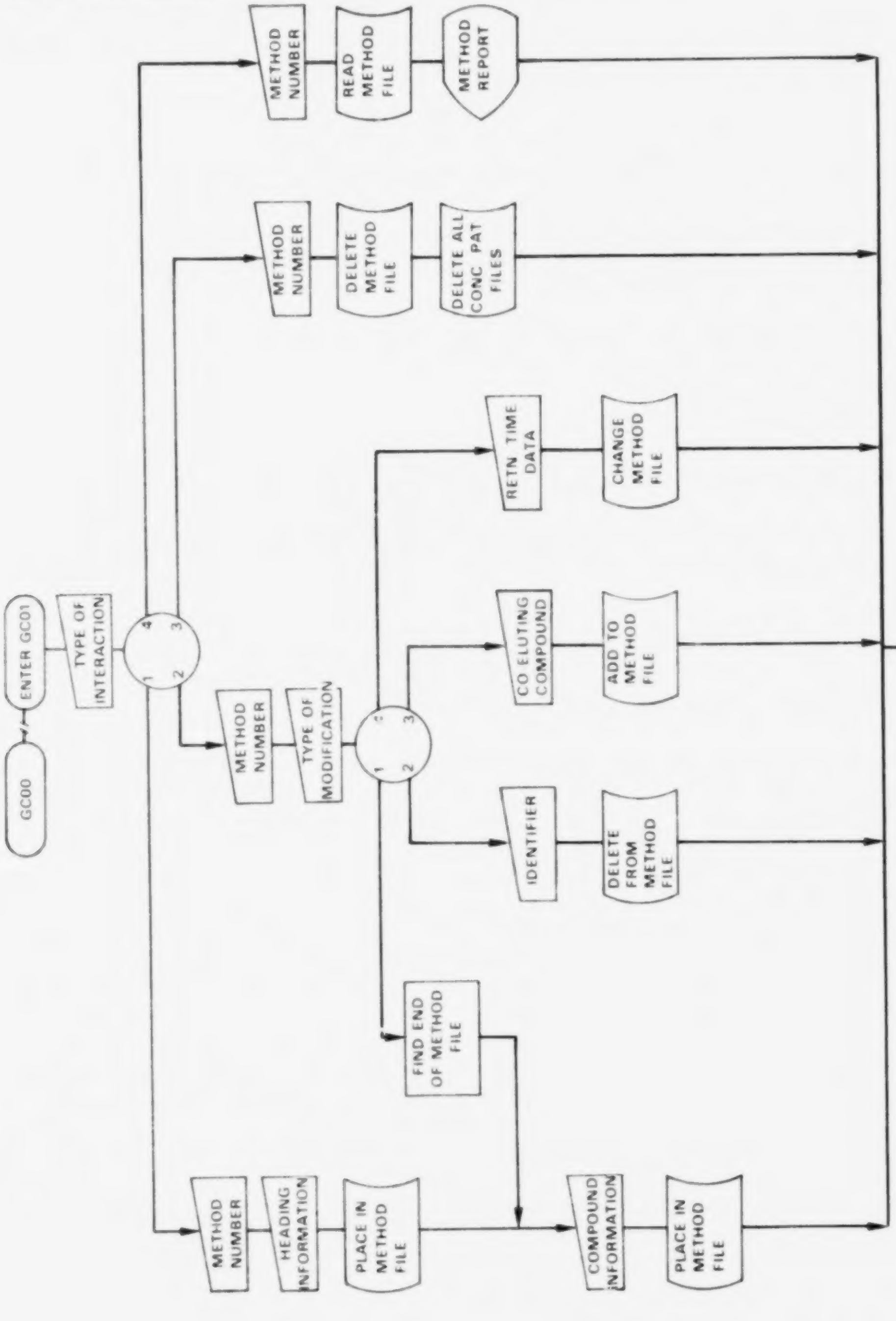

GC00
ENTER GC01
TYPE OF INTERACTION
1
2
3
4
METHOD NUMBER
READ METHOD FILE
METHOD REPORT
METHOD NUMBER
DELETE METHOD FILE
DELETE ALL CONC PAT FILES
METHOD NUMBER
TYPE OF MODIFICATION
1
2
3
4
RETN TIME DATA
CHANGE METHOD FILE
CO ELUTING COMPOUND
ADD TO METHOD FILE
IDENTIFIER
DELETE FROM METHOD FILE
FIND END OF METHOD FILE
METHOD NUMBER
HEADING INFORMATION
PLACE IN METHOD FILE
COMPOUND INFORMATION
PLACE IN METHOD FILE
CHAIN
GC00

Figure 3. Flowchart of Program GC01.

TABLE 2. SYMBOL DEFINITIONS FOR PROGRAM GC01

A6$	the name of a concentration pattern file
I	a record number counter and control variable for loops
I2	the control variable for loops
I3	the total in check digit calculations
I4	the control variable for a loop
J	the line number in method displays
N$	the identifier for the compound to whose retention time all others are relative, or the dead volume time
N1	the type of method N1=1 internal standards N1=2 purge and trap N1=3 liquid/liquid extraction N1=4 direct aqueous injection
N2	the type of retention time calculations N2=1 relative retention time N2=2 capacity ratio
T	the method number
T$	the name of the method file
U$	the user's name
V	the number of compounds associated with an identifier
V$	an identifier
V1$	the first compound associated with an identifier
V2$	the CAS number for V1$
V3$	the second compound associated with an identifier

TABLE 2. (continued)

V4$	the CAS number for V3$
V5$	the third compound associated with an identifier
V6$	the CAS number for V5$
V7$	the identifier to be modified
V8$	the additional compound to be associated with an identifier
V9$	the CAS number for V8$
W3$	a CAS number being sent to the subroutine
W4$	a CAS number padded with a space
X	the user's answer to a multiple choice question
X$	the user's answer to Y or N questions
X4	a dummy variable
X5	a dummy variable
Z5	the position of a slash in Z5$
Z5$	a string being sent to the subroutine to change slashes to commas

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  1
                    PROGRAM LISTING FOR GC01

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC01, METHOD GENERATION                         +
0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 26, 1979                +
0045 REM   +   MOST RECENT REVISION:  MARCH 26, 1979                   +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 4000
0090 DIM T$[6],U$[30],V$[8],V1$[40],V2$[11],V3$[40],V4$[11],V5$[40]
0100 DIM V6$[11],V7$[8],V8$[40],V9$[11],X$[3],W3$[11],W4$[11],N$[8]
0101 DIM Z5$[40],A6$[9]
0110 PRINT
0120 PRINT "HERE ARE THE TYPES OF METHOD INTERACTIONS:"
0130 PRINT
0140 PRINT "     1.  GENERATE A NEW METHOD"
0150 PRINT "     2.  MODIFY AN EXISTING METHOD"
0160 PRINT "     3.  DELETE AN EXISTING METHOD"
0170 PRINT "     4.  DISPLAY AN EXISTING METHOD"
0180 PRINT
0189 ON ERR THEN GOTO 0191
0190 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
0191 ON ERR THEN STOP
0200 ON X THEN GOTO 0260, 1750, 3120, 3370
0210 PRINT
0220 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
0230 GOTO 0110
0240 REM   ------------------------------------------------------------
0250 REM         GENERATE A NEW METHOD
0260 PRINT
0269 ON ERR THEN GOTO 0271
0270 INPUT "WHAT SHOULD BE THE NUMBER FOR THE NEW METHOD?  ",T
0271 ON ERR THEN STOP
0280 IF T=INT(ABS(T)) THEN IF T<=9999 THEN GOTO 0320
0290 PRINT
0300 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
0310 GOTO 0260
0320 LET T$="GC0000"
0330 LET T$[7-LEN(STR$(T)),6]=STR$(T)
0340 ON ERR THEN GOTO 0360
0350 RENAME T$,T$
0360 ON ERR THEN STOP

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  2
                    PROGRAM LISTING FOR GC01

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0370 IF SYS(7)<>-48 THEN GOTO 0400
0380 DELAY =1
0390 GOTO 0340
0400 IF SYS(7)<>-9 THEN GOTO 0480
0410 PRINT
0420 PRINT "<7><7>THERE IS AN EXISTING METHOD WITH THE NUMBER ";T$[3,6
*    ];"."
0430 PRINT "YOU MAY MODIFY METHOD ";T$[3,6];", OR YOU MAY DELETE IT AN
*    D THEN"
0440 PRINT "     GENERATE A NEW METHOD USING ";T$[3,6];" AS THE METHOD
*     NUMBER."
0450 PRINT "     HOWEVER, YOU MAY NOT GENERATE A SECOND METHOD WITH TH
*    E"
0460 PRINT "     SAME METHOD NUMBER."
0470 GOTO 0110
0480 OPEN FILE[4,0],T$,200
0490 ON ESC THEN GOTO 0510
0500 GOTO 0560
0510 CLOSE FILE[4]
0520 PRINT
0530 PRINT "<7><7>METHOD ";T$[3,6];" HAS BEEN DELETED BECAUSE IT WAS I
*    NCOMPLETE."
0540 DELETE T$
0550 GOTO 4000
0560 PRINT
0570 ON ERR THEN GOTO 0590
0580 INPUT "WHAT IS YOUR NAME?  ",U$
0581 ON ERR THEN STOP
0582 LET Z5$=U$
0583 GOSUB 4370
0584 LET U$=Z5$
0585 GOTO 0600
0590 ON ERR THEN STOP
0591 PRINT
0592 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
0593 GOTO 0560
0600 PRINT
0610 PRINT "HERE ARE THE TYPES OF METHODS:"
0620 PRINT
0630 PRINT "     1.  INTERNAL STANDARDS"
0640 PRINT "     2.  PURGE AND TRAP"
0650 PRINT "     3.  LIQUID/LIQUID EXTRACTION"

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  3
                     PROGRAM LISTING FOR GC01

1234567891123456789212345678931234567894123456789512345678961234567897
         0          0          0          0          0          0      0
0660 PRINT "     4.  DIRECT AQUEOUS INJECTION"
0670 PRINT
0679 ON ERR THEN GOTO 0681
0680 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",N1
0681 ON ERR THEN STOP
0690 IF INT(ABS(N1))=N1 THEN IF N1>0 THEN IF N1<5 THEN GOTO 0730
0700 PRINT
0710 PRINT "<7><7>";N1;"IS NOT A VALID TYPE NUMBER."
0720 GOTO 0600
0730 PRINT
0740 PRINT "HERE ARE THE TYPES OF RETENTION TIME CALCULATIONS:"
0750 PRINT
0760 PRINT "     1.  RELATIVE RETENTION TIME"
0770 PRINT "     2.  CAPACITY RATIO"
0780 PRINT
0789 ON ERR THEN GOTO 0791
0790 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1 OR 2)  ",N2
0791 ON ERR THEN STOP
0800 PRINT
0810 IF N2=1 THEN GOTO 0850
0820 IF N2=2 THEN GOTO 0880
0830 PRINT "<7><7>";N2;"IS NOT A VALID TYPE NUMBER."
0840 GOTO 0730
0850 PRINT "WHAT IS THE IDENTIFIER FOR THE REFERENCE COMPOUND FOR"
0851 ON ERR THEN GOTO 0860
0852 INPUT "     RELATIVE RETENTION TIMES?  ",N$
0853 ON ERR THEN STOP
0854 LET Z5$=N$
0855 GOSUB 4370
0856 LET N$=Z5$
0857 GOTO 0890
0860 ON ERR THEN STOP
0861 PRINT
0862 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
0863 PRINT
0864 GOTO 0850
0880 ON ERR THEN GOTO 0882
0881 INPUT "WHAT IS THE DEAD VOLUME TIME, IN SECONDS?  ",N$
0882 ON ERR THEN GOTO 0886
0883 LET X4=VAL(N$)
0884 ON ERR THEN STOP
0885 GOTO 0890

1234567891123456789212345678931234567894123456789512345678961234567897
         0          0          0          0          0          0      0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  4
                     PROGRAM LISTING FOR GC01

1234567891123456789212345678931234567894123456789512345678961234567897
         0          0          0          0          0          0      0
0886 ON ERR THEN STOP
0887 PRINT
0888 PRINT "<7><7>";N$;" IS NOT A VALID DEAD VOLUME TIME."
0889 GOTO 0800
0890 WRITE FILE[4,1],T$,U$,N1,N2,N$
0900 GOTO 0910
0910 LET I=1
0920 PRINT
0930 PRINT "ENTER THE FOLLOWING COMPOUND IDENTIFICATION INFORMATION."
0940 PRINT "USE A SLASH (/) WHERE YOU WANT A COMMA."
0950 PRINT "TYPE 'END' AS AN IDENTIFIER TO TERMINATE THE LIST."
0960 IF I<=60 THEN GOTO 1010
0970 PRINT
0980 PRINT "<7><7>YOU HAVE ENTERED 60 IDENTIFIERS, WHICH IS THE LIMIT"
0990 PRINT "     FOR THIS PROGRAM."
1000 GOTO 1660
1010 LET V3$="99999"
1020 LET V4$="99999"
1030 LET V5$="99999"
1040 LET V6$="99999"
1050 PRINT
1060 ON ERR THEN GOTO 1080
1070 INPUT "IDENTIFIER?  ",V$
1071 ON ERR THEN STOP
1072 LET Z5$=V$
1073 GOSUB 4370
1074 LET V$=Z5$
1075 GOTO 1090
1080 PRINT
1082 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
1083 GOTO 1050
1090 IF V$="END" THEN GOTO 1660
1099 ON ERR THEN GOTO 1101
1100 INPUT "     NUMBER OF COMPOUNDS?  (1, 2, OR 3)  ",V
1101 ON ERR THEN STOP
1110 IF V=INT(ABS(V)) THEN IF V>0 THEN IF V<4 THEN GOTO 1170
1130 PRINT "<7><7>     ";V;"IS NOT A VALID NUMBER OF COMPOUNDS."
1150 GOTO 1100
1170 PRINT "     NAME OF ";
1180 IF V<>1 THEN PRINT "FIRST ";
1189 ON ERR THEN GOTO 1200
1190 INPUT "COMPOUND?  ",V1$

1234567891123456789212345678931234567894123456789512345678961234567897
         0          0          0          0          0          0      0
```

PROGRAM LISTING FOR GC01

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1191 ON ERR THEN STOP
1192 LET Z5$=V1$
1193 GOSUB 4370
1194 LET V1$=Z5$
1195 GOTO 1210
1200 ON ERR THEN STOP
1201 PRINT
1202 PRINT "<7><7>     USE A SLASH (/) WHERE YOU WANT A COMMA."
1204 GOTO 1170
1210 ON ERR THEN GOTO 1230
1220 INPUT "          CAS NUMBER?  ",V2$
1230 ON ERR THEN STOP
1240 IF LEN(V2$)=0 THEN GOTO 1320
1250 LET W3$=V2$
1260 GOSUB 4050
1270 IF W3$<>"99999" THEN GOTO 1310
1290 PRINT "<7><7>          ";V2$;" IS NOT A VALID CAS NUMBER."
1300 GOTO 1210
1310 LET V2$=W3$
1320 IF V<2 THEN GOTO 1620
1330 ON ERR THEN GOTO 1350
1340 INPUT "     NAME OF SECOND CUMPOUND?  ",V3$
1341 ON ERR THEN STOP
1342 LET Z5$=V3$
1343 GOSUB 4370
1344 LET V3$=Z5$
1345 GOTO 1360
1350 ON ERR THEN STOP
1351 PRINT
1352 PRINT "<7><7>     USE A SLASH (/) WHERE YOU WANT A COMMA."
1354 GOTO 1330
1360 ON ERR THEN GOTO 1380
1370 INPUT "          CAS NUMBER?  ",V4$
1380 ON ERR THEN STOP
1390 IF LEN(V4$)=0 THEN GOTO 1470
1400 LET W3$=V4$
1410 GOSUB 4050
1420 IF W3$<>"99999" THEN GOTO 1460
1440 PRINT "<7><7>          ";V4$;" IS NOT A VALID CAS NUMBER."
1450 GOTO 1360
1460 LET V4$=W3$
1470 IF V<3 THEN GOTO 1620

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC01

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1480 ON ERR THEN GOTO 1500
1490 INPUT "     NAME OF THIRD COMPOUND?  ",V5$
1491 ON ERR THEN STOP
1492 LET Z5$=V5$
1493 GOSUB 4370
1494 LET V5$=Z5$
1495 GOTO 1510
1500 ON ERR THEN STOP
1501 PRINT
1502 PRINT "<7><7>     USE A SLASH (/) WHERE YOU WANT A COMMA."
1504 GOTO 1480
1510 ON ERR THEN GOTO 1530
1520 INPUT "          CAS NUMBER?  ",V6$
1530 ON ERR THEN STOP
1540 IF LEN(V6$)=0 THEN GOTO 1620
1550 LET W3$=V6$
1560 GOSUB 4050
1570 IF W3$<>"99999" THEN GOTO 1610
1590 PRINT "<7><7>          ";V6$;" IS NOT A VALID CAS NUMBER."
1600 GOTO 1510
1610 LET V6$=W3$
1620 WRITE FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
1630 WRITE FILE[4,3*I],"99/99/99","",99999,99999,99999,99999,99999
1640 LET I=I+1
1650 GOTO 0960
1660 CLOSE FILE[4]
1670 PRINT
1680 ON ERR THEN GOTO 1700
1690 INPUT "DO YOU WANT TO DISPLAY THIS METHOD?  (Y OR N)  ",X$
1700 ON ERR THEN STOP
1710 IF X$[1,1]="Y" THEN GOTO 3550
1720 GOTO 4000
1730 REM  ------------------------------------------------------------
1740 REM          MODIFY AN EXISTING METHOD
1750 PRINT
1759 ON ERR THEN GOTO 1761
1760 INPUT "WHICH METHOD DO YOU WANT TO MODIFY?  ",T
1761 ON ERR THEN STOP
1770 IF ABS(INT(T))=T THEN IF T<=9999 THEN GOTO 1810
1780 PRINT
1790 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
1800 GOTO 1750

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  7
                       PROGRAM LISTING FOR GC01

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 1810 LET T$="GC0000"
 1820 LET T$[7-LEN(STR$(T)),6]=STR$(T)
 1830 ON ERR THEN GOTO 1850
 1840 RENAME T$,T$
 1850 ON ERR THEN STOP
 1860 IF SYS(7)<>-48 THEN GOTO 1890
 1870 DELAY =1
 1880 GOTO 1830
 1890 IF SYS(7)=-9 THEN GOTO 1950
 1900 PRINT
 1910 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*     ];"."
 1920 PRINT "NO METHOD HAS BEEN MODIFIED."
 1930 GOTO 3950
 1940 PRINT
 1950 ON ERR THEN GOTO 1990
 1960 OPEN FILE[4,0],T$,200
 1970 ON ERR THEN STOP
 1980 GOTO 2020
 1990 ON ERR THEN STOP
 2000 DELAY =1
 2010 GOTO 1950
 2020 PRINT
 2030 PRINT "HERE ARE THE TYPES OF METHOD MODIFICATION:"
 2040 PRINT
 2050 PRINT "     1.  ADD AN IDENTIFIER"
 2060 PRINT "     2.  DELETE AN IDENTIFIER"
 2070 PRINT "     3.  ADD ANOTHER CO-ELUTING COMPOUND TO THE LIST FOR A
*     N IDENTIFIER"
 2080 PRINT "     4.  CHANGE RETENTION TIME DATA"
 2090 PRINT
 2099 ON ERR THEN GOTO 2101
 2100 INPUT "WHICH TYPE TO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
 2101 ON ERR THEN STOP
 2110 ON X THEN GOTO 2170, 2270, 2460, 2910
 2120 PRINT
 2130 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
 2140 GOTO 2020
 2150 REM  ------------------------------------
 2160 REM     ADD ANOTHER IDENTIFIER
 2170 NOESC
 2171 GOSUB 4430

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  8
                       PROGRAM LISTING FOR GC01

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 2172 ESC
 2173 PRINT
 2174 PRINT "ALL CONCENTRATION PATTERNS FOR METHOD ";T$[3,6];" HAVE BEE
*     N DELETED."
 2175 LET I=1
 2180 READ FILE[4,3*I-1],V$
 2190 IF EOF(4) THEN GOTO 2220
 2200 LET I=I+1
 2210 GOTO 2180
 2220 PRINT
 2230 PRINT "ENTER THE COMPOUND IDENTIFICATION INFORMATION FOR THE NEW
*     IDENTIFIER."
 2240 GOTO 0940
 2250 REM  ------------------------------------
 2260 REM     DELETE AN IDENTIFIER
 2270 PRINT
 2280 ON ERR THEN GOTO 2300
 2290 INPUT "WHICH IDENTIFIER DO YOU WANT TO DELETE?  ",V7$
 2291 ON ERR THEN STOP
 2292 LET Z5$=V7$
 2293 GOSUB 4370
 2294 LET V7$=Z5$
 2295 GOTO 2310
 2300 ON ERR THEN STOP
 2301 PRINT
 2302 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
 2303 GOTO 2270
 2310 LET I=1
 2320 READ FILE[4,3*I-1],V$
 2330 IF EOF(4) THEN GOTO 2370
 2340 IF V$=V7$ THEN GOTO 2400
 2350 LET I=I+1
 2360 GOTO 2320
 2370 PRINT
 2380 PRINT "<7><7>THERE IS NO IDENTIFIER ";V7$;" IN METHOD ";T$[3,6];"
*     ."
 2390 GOTO 3930
 2400 WRITE FILE[4,3*I-1],"99999","99999","99999","99999","99999","9999
*     9","99999"
 2410 PRINT
 2420 PRINT "IDENTIFIER ";V7$;" HAS BEEN DELETED FROM METHOD ";T$[3,6]
 2430 GOTO 3930

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC01

```
12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
2440 REM  ----------------------------------------
2450 REM     ADD ANOTHER COMPOUND TO AN IDENTIFIER
2460 PRINT
2470 ON ERR THEN GOTO 2490
2480 INPUT "WHICH IDENTIFIER DO YOU WANT TO ADD TO?  ",V7$
2481 ON ERR THEN STOP
2482 LET Z5$=V7$
2483 GOSUB 4370
2484 LET V7$=Z5$
2485 GOTO 2500
2490 ON ERR THEN STOP
2491 PRINT
2492 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
2493 GOTO 2460
2500 LET I=1
2510 READ FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
2520 IF EOF(4) THEN GOTO 2560
2530 IF V$=V7$ THEN GOTO 2600
2540 LET I=I+1
2550 GOTO 2510
2560 PRINT
2570 PRINT "<7><7>THERE IS NO IDENTIFIER ";V7$;" IN METHOD ";T$[3,6];"
*    ."
2580 PRINT "NO IDENTIFIER HAS BEEN CHANGED."
2590 GOTO 3930
2600 IF V5$="99999" THEN GOTO 2640
2610 PRINT
2620 PRINT "<7><7>";V7$;" ALREADY HAS THE LIMIT OF THREE CO-ELUTING CO
*    MPOUNDS."
2630 GOTO 3930
2640 PRINT
2650 ON ERR THEN GOTO 2670
2660 INPUT "WHAT IS THE NAME OF THE ADDITIONAL CO-ELUTING COMPOUND?  "
*    ,V8$
2661 ON ERR THEN STOP
2662 LET Z5$=V8$
2663 GOSUB 4370
2664 LET V8$=Z5$
2665 GOTO 2680
2670 ON ERR THEN STOP
2671 PRINT
2672 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."

12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
```

PROGRAM LISTING FOR GC01

```
12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
2673 GOTO 2640
2680 PRINT
2690 PRINT "WHAT IS THE CAS NUMBER FOR ";V8$;
2700 ON ERR THEN GOTO 2720
2710 INPUT "?  ",V9$
2720 ON ERR THEN STOP
2730 IF LEN(V9$)=0 THEN GOTO 2810
2740 LET W3$=V9$
2750 GOSUB 4050
2760 IF W3$<>"99999" THEN GOTO 2800
2770 PRINT
2780 PRINT "<7><7>";V9$;" IS NOT A VALID CAS NUMBER."
2790 GOTO 2680
2800 LET V9$=W3$
2810 IF V3$<>"99999" THEN GOTO 2850
2820 LET V3$=V8$
2830 LET V4$=V9$
2840 GOTO 2870
2850 LET V5$=V8$
2860 LET V6$=V9$
2870 WRITE FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
2880 GOTO 3930
2890 REM  ----------------------------------------
2900 REM     CHANGE RETENTION TIME DATA
2910 PRINT
2920 PRINT "HERE ARE THE TYPES OF RETENTION TIME CALCULATIONS:"
2930 PRINT
2940 PRINT "     1. RELATIVE RETENTION TIME"
2950 PRINT "     2. CAPACITY RATIO"
2960 PRINT
2969 ON ERR THEN GOTO 2971
2970 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1 OR 2)  ",N2
2971 ON ERR THEN STOP
2980 PRINT
2990 IF N2=1 THEN GOTO 3030
3000 IF N2=2 THEN GOTO 3060
3010 PRINT "<7><7>";N2;"IS NOT A VALID TYPE NUMBER."
3020 GOTO 2910
3030 PRINT "WHAT IS THE IDENTIFIER FOR THE REFERENCE COMPOUND FOR"
3031 ON ERR THEN GOTO 3040
3032 INPUT "     RELATIVE RETENTION TIMES?  ",N$
3033 ON ERR THEN STOP

12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
```

```
12345678911234567892123456789312345678941234567895123456789612345678970
        0         0         0         0         0         0         0
3034 LET Z5$=N$
3035 GOSUB 4370
3036 LET N$=Z5$
3037 GOTO 3070
3040 ON ERR THEN STOP
3041 PRINT
3042 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
3043 PRINT
3044 GOTO 3030
3060 ON ERR THEN GOTO 3062
3061 INPUT "WHAT IS THE DEAD VOLUME TIME, IN SECONDS?  ",N$
3062 ON ERR THEN GOTO 3066
3063 LET X5=VAL(N$)
3064 ON ERR THEN STOP
3065 GOTO 3070
3066 ON ERR THEN STOP
3067 PRINT
3068 PRINT "<7><7>";N$;" IS NOT A VALID DEAD VOLUME TIME."
3069 GOTO 2980
3070 READ FILE[4,1],T$,U$,N1
3080 WRITE FILE[4,1],T$,U$,N1,N2,N$
3090 GOTO 3930
3100 REM   ------------------------------------------------------------
3110 REM          DELETE AN EXISTING METHOD
3120 PRINT
3129 ON ERR THEN GOTO 3131
3130 INPUT "WHICH METHOD DO YOU WANT TO DELETE?  ",T
3131 ON ERR THEN STOP
3140 IF T=INT(ABS(T)) THEN IF T<=9999 THEN GOTO 3180
3150 PRINT
3160 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
3170 GOTO 3120
3180 LET T$="GC0000"
3190 LET T$[7-LEN(STR$(T)),6]=STR$(T)
3200 ON ERR THEN GOTO 3220
3210 RENAME T$,T$
3220 ON ERR THEN STOP
3230 IF SYS(7)<>-48 THEN GOTO 3260
3240 DELAY =1
3250 GOTO 3200
3260 IF SYS(7)=-9 THEN GOTO 3310
3270 PRINT

12345678911234567892123456789312345678941234567895123456789612345678970
        0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678970
        0         0         0         0         0         0         0
3280 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*     ];"."
3290 PRINT "NO METHOD HAS BEEN DELETED."
3300 GOTO 3950
3310 NOESC
3311 DELETE T$
3312 GOSUB 4430
3313 ESC
3320 PRINT
3330 PRINT "METHOD ";T$[3,6];" AND ALL OF ITS CONCENTRATION PATTERNS H
*     AVE BEEN DELETED."
3340 GOTO 3950
3350 REM   ------------------------------------------------------------
3360 REM          DISPLAY AN EXISTING METHOD
3370 PRINT
3379 ON ERR THEN GOTO 3381
3380 INPUT "WHAT METHOD DO YOU WANT TO DISPLAY?  ",T
3381 ON ERR THEN STOP
3390 IF T=INT(ABS(T)) THEN IF T<=9999 THEN GOTO 3430
3400 PRINT
3410 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
3420 GOTO 3370
3430 LET T$="GC0000"
3440 LET T$[7-LEN(STR$(T)),6]=STR$(T)
3450 ON ERR THEN GOTO 3470
3460 RENAME T$,T$
3470 ON ERR THEN STOP
3480 IF SYS(7)<>-48 THEN GOTO 3510
3490 DELAY =1
3500 GOTO 3450
3510 IF SYS(7)=-9 THEN GOTO 3550
3520 PRINT
3530 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*     ];"."
3540 GOTO 3950
3550 ON ERR THEN GOTO 3590
3560 OPEN FILE[4,0],T$,200
3570 ON ERR THEN STOP
3580 GOTO 3620
3590 ON ERR THEN STOP
3600 DELAY =1
3610 GOTO 3550

12345678911234567892123456789312345678941234567895123456789612345678970
        0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE 13
                        PROGRAM LISTING FOR GC01

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
 3620 PRINT
 3630 READ FILE[4,1],T$,U$,N1,N2,N$
 3635 PRINT
 3636 PRINT
 3637 PRINT  TAB(24);"M-E-T-H-O-D  R-E-P-O-R-T"
 3638 PAGE =74
 3640 PRINT "ANALYST:  ";U$; TAB(53);"METHOD NUMBER:  ";T$[3,6]
 3660 PRINT "TYPE OF METHOD:  ";
 3670 ON N1 THEN GOTO 3680, 3700, 3720, 3740
 3680 PRINT "INTERNAL STANDARDS"
 3690 GOTO 3750
 3700 PRINT "PURGE AND TRAP "
 3710 GOTO 3750
 3720 PRINT "LIQUID/LIQUID EXTRACTION"
 3730 GOTO 3750
 3740 PRINT "DIRECT AQUEOUS INJECTION"
 3750 UN N2 THEN GOTO 3760, 3780
 3760 PRINT "IDENTIFIER FOR RELATIVE RETENTION TIME REFERENCE PEAK:  ";
*     N$
 3770 GOTO 3790
 3780 PRINT "DEAD VOLUME TIME FOR CAPACITY RATIOS:  ";N$;" SECONDS"
 3790 PRINT
 3800 PRINT "    IDENTIFIER                 NAME OF COMPOUND
*        CAS NUMBER"
 3810 PRINT "    ----------  ---------------------------------------
*     -----------"
 3820 LET I=1
 3830 LET J=0
 3840 READ FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
 3850 IF EOF(4) THEN GOTO 3930
 3860 IF V$="99999" THEN GOTO 3910
 3870 LET J=J+1
 3880 PRINT USING "###.  ########    ###############################
*     #######  ###########",J,V$,V1$,V2$
 3890 IF V3$<>"99999" THEN PRINT USING "                   #############
*     #############################  ###########",V3$,V4$
 3900 IF V5$<>"99999" THEN PRINT USING "                   #############
*     #############################  ###########",V5$,V6$
 3910 LET I=I+1
 3920 GOTO 3840
 3930 CLOSE FILE[4]
 3940 ON ESC THEN GOTO 4000

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE 14
                        PROGRAM LISTING FOR GC01

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
 3950 PRINT
 3955 PRINT
 3960 ON ERR THEN GOTO 3980
 3970 INPUT "DO YOU WANT TO DEAL FURTHER WITH ANY METHOD?  (Y OR N)  ",
*     X$
 3980 ON ERR THEN STOP
 3990 IF X$[1,1]="Y" THEN GOTO 0110
 4000 CLOSE
 4010 NOESC
 4020 CHAIN "GC00" THEN GOTO 0100
 4040 REM
 4050 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 4060 REM          SUBROUTINE TO CHECK VALIDITY OF CAS NUMBERS
 4070 IF LEN(W3$)=11 THEN GOTO 4110
 4080 LET W4$=" ",W3$
 4090 LET W3$=W4$
 4100 GOTO 4070
 4110 IF W3$[7,7]="-" THEN IF W3$[10,10]="-" THEN GOTO 4130
 4120 GOTO 4310
 4130 LET I3=0
 4140 FOR I4=1 TO 6
 4150   IF W3$[I4,I4]<>" " THEN GOTO 4170
 4160 NEXT I4
 4170 FOR I2=I4 TO 6
 4180   ON ERR THEN GOTO 4310
 4190   LET I3=I3+VAL(W3$[I2,I2])*(9-I2)
 4200   ON ERR THEN STOP
 4210 NEXT I2
 4220 FOR I2=8 TO 9
 4230   ON ERR THEN GOTO 4310
 4240   LET I3=I3+VAL(W3$[I2,I2])*(10-I2)
 4250   ON ERR THEN STOP
 4260 NEXT I2
 4270 ON ERR THEN GOTO 4310
 4280 IF I3-10*INT(I3/10)<>VAL(W3$[11,11]) THEN GOTO 4310
 4290 ON ERR THEN STOP
 4300 RETURN
 4310 ON ERR THEN STOP
 4320 LET W3$="99999"
 4330 RETURN
 4340 REM
 4350 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE 15
                       PROGRAM LISTING FOR GC01

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
4360 REM          SUBROUTINE TO CHANGE SLASHES TO COMMAS
4370 LET Z5=POS(Z5$,"/",1)
4380 IF Z5=0 THEN RETURN
4390 LET Z5$[Z5,Z5]=","
4400 GOTO 4370
4405 REM
4410 REM   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
4420 REM          SUBROUTINE TO DELETE CONCENTRATION PATTERNS
4430 LET A6$=T$,"000"
4440 FOR I=1 TO 26
4450   LET A6$[10-LEN(STR$(I)),9]=STR$(I)
4460   ON ERR THEN GOTO 4480
4470   DELETE A6$
4480   ON ERR THEN STOP
4490 NEXT I
4500 RETURN

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE 16
                        SYMBOL TABLE FOR GC01

SYMBOL    REFERENCES
------  ------------------------------------------------------------
 0100   4020
 0110   0230  0470  3990
 0191   0189
 0260   0200  0310
 0271   0269
 0320   0280
 0340   0390
 0360   0340
 0400   0370
 0480   0400
 0510   0490
 0560   0500  0593
 0590   0570
 0600   0585  0720
 0681   0679
 0730   0690  0840
 0791   0789
 0800   0889
 0850   0810  0864
 0860   0851
 0880   0820
 0882   0880
 0886   0882
 0890   0857  0885
 0910   0900
 0940   2240
 0960   1650
 1010   0960
 1050   1083
 1080   1060
 1090   1075
 1100   1150
 1101   1099
 1170   1110  1204
 1200   1189
 1210   1195  1300
 1230   1210
 1310   1270
 1320   1240
 1330   1354
 1350   1330
 1360   1345  1450
 1380   1360
 1460   1420
 1470   1390
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE 17
                         SYMBOL TABLE FOR GC01

SYMBOL    REFERENCES
------  ----------------------------------------------------------------
  1480  1504
  1500  1480
  1510  1495  1600
  1530  1510
  1610  1570
  1620  1320  1470  1540
  1660  1000  1090
  1700  1680
  1750  0200  1800
  1761  1759
  1810  1770
  1830  1880
  1850  1830
  1890  1860
  1950  1890  2010
  1990  1950
  2020  1980  2140
  2101  2099
  2170  2110
  2180  2210
  2220  2190
  2270  2110  2303
  2300  2280
  2310  2295
  2320  2360
  2370  2330
  2400  2340
  2460  2110  2493
  2490  2470
  2500  2485
  2510  2550
  2560  2520
  2600  2530
  2640  2600  2673
  2670  2650
  2680  2665  2790
  2720  2700
  2800  2760
  2810  2730
  2850  2810
  2870  2840
  2910  2110  3020
  2971  2969
  2980  3069
  3030  2990  3044
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE 18
                         SYMBOL TABLE FOR GC01

SYMBOL    REFERENCES
------  ----------------------------------------------------------------
  3040  3031
  3060  3000
  3062  3060
  3066  3062
  3070  3037  3065
  3120  0200  3170
  3131  3129
  3180  3140
  3200  3250
  3220  3200
  3260  3230
  3310  3260
  3370  0200  3420
  3381  3379
  3430  3390
  3450  3500
  3470  3450
  3510  3480
  3550  1710  3510  3610
  3590  3550
  3620  3580
  3680  3670
  3700  3670
  3720  3670
  3740  3670
  3750  3690  3710  3730
  3760  3750
  3780  3750
  3790  3770
  3840  3920
  3910  3860
  3930  2390  2430  2590  2630  2880  3090  3850
  3950  1930  3300  3340  3540
  3980  3960
  4000  0080  0550  1720  3940
  4050  1260  1410  1560  2750
  4070  4100
  4110  4070
  4130  4110
  4170  4150
  4310  4120  4180  4230  4270  4280
  4370  0583  0855  1073  1193  1343  1493  2293  2483  2663  3035
        4400
  4430  2171  3312
  4480  4460
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE 19
                         SYMBOL TABLE FOR GC01

SYMBOL    REFERENCES
------  ---------------------------------------------------------------
 A6$    0101  4430  4450  4470
 FL#4   0480  0510  0890  1620  1630  1660  1960  2180  2320  2400
        2510  2870  3070  3080  3560  3630  3840  3930
 I      0910  0960  1620  1630  1640  2175  2180  2200  2310  2320
        2350  2400  2500  2510  2540  2870  3820  3840  3910  4440
        4450  4490
 I2     4170  4190  4210  4220  4240  4260
 I3     4130  4190  4240  4290
 I4     4140  4150  4160  4170
 J      3830  3870  3880
 N$     0100  0852  0854  0856  0881  0883  0888  0890  3032  3034
        3036  3061  3063  3068  3080  3630  3760  3780
 N1     0680  0690  0710  0890  3070  3080  3630  3670
 N2     0790  0810  0820  0830  0890  2970  2990  3000  3010  3080
        3630  3750
 T      0270  0280  0300  0330  1760  1770  1790  1820  3130  3140
        3160  3190  3380  3390  3410  3440
 T$     0090  0320  0330  0350  0420  0430  0440  0480  0530  0540
        0890  1810  1820  1840  1910  1960  2174  2380  2420  2570
        3070  3080  3180  3190  3210  3280  3311  3330  3430  3440
        3460  3530  3560  3630  3640  4430
 U$     0090  0580  0582  0584  0890  3070  3080  3630  3640
 V      1100  1110  1130  1180  1320  1470
 V$     0090  1070  1072  1074  1090  1620  2180  2320  2340  2510
        2530  2870  3840  3860  3880
 V1$    0090  1190  1192  1194  1620  2510  2870  3840  3880
 V2$    0090  1220  1240  1250  1290  1310  1620  2510  2870  3840
        3880
 V3$    0090  1010  1340  1342  1344  1620  2510  2810  2820  2870
        3840  3890
 V4$    0090  1020  1370  1390  1400  1440  1460  1620  2510  2830
        2870  3840  3890
 V5$    0090  1030  1490  1492  1494  1620  2510  2600  2850  2870
        3840  3900
 V6$    0100  1040  1520  1540  1550  1590  1610  1620  2510  2860
        2870  3840  3900
 V7$    0100  2290  2292  2294  2340  2380  2420  2480  2482  2484
        2530  2570  2620
 V8$    0100  2660  2662  2664  2690  2820  2850
 V9$    0100  2710  2730  2740  2780  2800  2830  2860
 W3$    0100  1250  1270  1310  1400  1420  1460  1550  1570  1610
        2740  2760  2800  4070  4080  4090  4110  4150  4190  4240
        4280  4320
 W4$    0100  4080  4090
 X      0190  0200  0220  2100  2110  2130
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE 20
                         SYMBOL TABLE FOR GC01

SYMROL    REFERENCES
------  ---------------------------------------------------------------
 X$     0100  1690  1710  3970  3990
 X4     0883
 X5     3063
 Z5     4370  4380  4390
 Z5$    0101  0582  0584  0854  0856  1072  1074  1192  1194  1342
        1344  1492  1494  2292  2294  2482  2484  2662  2664  3034
        3036  4370  4390
```

SECTION 4

PROGRAM GC02 - CONCENTRATION PATTERN INTERACTION

GC02 is the program which creates, deletes, displays, and lists the names of concentration patterns. It is entered by chaining from the master control program, GC00, and it returns control to that program if the escape key is pressed.

The functions of this program are relatively simple. It first gives the user the choice of the four possible actions and then branches to the appropriate routine.

To create a concentration pattern file, the program loops through the method file and asks the user for the prepared concentration for each identifier. It places these concentrations in the concentration pattern file named by the user.

To delete an existing pattern, the program simply asks the user for the name of the pattern and deletes that file.

To display an existing pattern, the program loops through the method file and the concentration pattern file simultaneously and prints the identifiers and their associated concentrations.

To list the names of the existing concentration patterns, the program checks each of the 26 possible concentration pattern file names to see if such a file exists. It prints the names of those which do exist.

At the end of this program, it chains back to GC00.

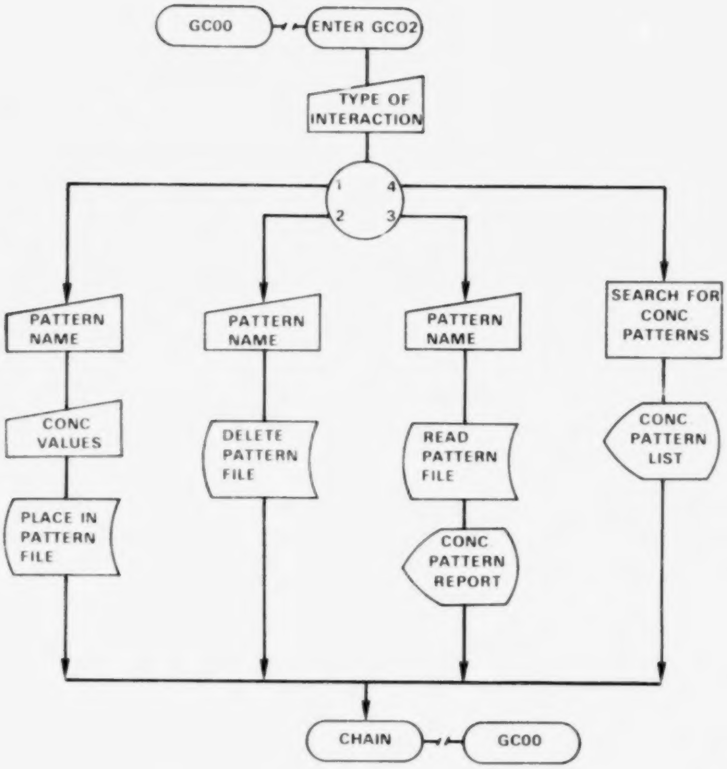

GC00
ENTER GC02
TYPE OF INTERACTION
1
2
3
4
PATTERN NAME
CONC VALUES
PLACE IN PATTERN FILE
PATTERN NAME
DELETE PATTERN FILE
PATTERN NAME
READ PATTERN FILE
CONC PATTERN REPORT
SEARCH FOR CONC PATTERNS
CONC PATTERN LIST
CHAIN
GC00

Figure 4. Flowchart of Program GC02.

TABLE 3. SYMBOL DEFINITIONS FOR PROGRAM GC02

A5	the prepared concentration input by the user
A6$	the name of the concentration pattern file
A7	the position of A8$ in A9$
A8$	the single letter name of a concentration pattern
A9$	the alphabet
I	the control variable for loops
I2	a counter for the number of concentration patterns associated with a method
T$	the name of the method file
V$	an identifier from the method file
X	the user's answer to multiple choice questions
X$	the user's answer to Y or N questions

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                        PROGRAM LISTING FOR GC02

 1234567891123456789212345678931234567894123456789512345678961234567897
          0          0          0          0          0          0          0
 0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                      +
 0030 REM   +   PROGRAM GC02, CONCENTRATION PATTERN INTERACTION           +
 0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 23, 1979                    +
 0050 REM   +   MOST RECENT REVISION:  MAY 18, 1979                       +
 0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0070 REM
 0080 ON ESC THEN GOTO 1830
 0090 ESC
 0100 DIM A6$[9],A8$[1],A9$[26],T$[6],V$[8],X$[3]
 0110 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
 0120 READ FILE[4,1],T$
 0130 REM   ---------------------------------------------------------------
 0140 REM            DISPLAY CHOICES
 0150 PRINT
 0160 PRINT "HERE ARE THE TYPES OF CONCENTRATION PATTERN INTERACTION FO
*     R METHOD ";T$[3,6];":"
 0170 PRINT
 0180 PRINT "      1.   CREATE A NEW CONCENTRATION PATTERN"
 0190 PRINT "      2.   DELETE AN EXISTING PATTERN"
 0200 PRINT "      3.   DISPLAY AN EXISTING PATTERN"
 0210 PRINT "      4.   LIST THE EXISTING PATTERNS FOR METHOD ";T$[3,6]
 0220 PRINT
 0230 ON ERR THEN GOTO 0250
 0240 INPUT "WHAT TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
 0250 ON ERR THEN STOP
 0260 IF X=INT(X) THEN IF X>0 THEN IF X<5 THEN GOTO 0300
 0270 PRINT
 0280 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
 0290 GOTO 0150
 0300 ON X THEN GOTO 0330, 0820, 1050, 1530
 0310 REM   ---------------------------------------------------------------
 0320 REM            CREATE A NEW CONCENTRATION PATTERN FILE
 0330 PRINT
 0340 ON ERR THEN GOTO 0360
 0350 INPUT "WHAT SHOULD BE THE LETTER NAME FOR THE NEW PATTERN?  (A, B
*     , C, . . . , OR Z)  ",A8$
 0360 ON ERR THEN STOP
 0370 LET A7=POS(A9$,A8$,1)
 0380 IF A7<>0 THEN GOTO 0420
 0390 PRINT
 0400 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."

 1234567891123456789212345678931234567894123456789512345678961234567897
          0          0          0          0          0          0          0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                        PROGRAM LISTING FOR GC02

 1234567891123456789212345678931234567894123456789512345678961234567897
          0          0          0          0          0          0          0
 0410 GOTO 0330
 0420 LET A6$=T$,"000"
 0430 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
 0440 ON ERR THEN GOTO 0460
 0450 RENAME A6$,A6$
 0460 ON ERR THEN STOP
 0470 IF SYS(7)=-10 THEN GOTO 0510
 0480 PRINT
 0490 PRINT "<7><7>THERE IS ALREADY A PATTERN NAMED '";A8$;"' FOR METHO
*     D ";T$[3,6];"."
 0500 GOTO 0330
 0510 OPEN FILE[7,0],A6$,4
 0520 ON ESC THEN GOTO 0540
 0530 GOTO 0590
 0540 CLOSE FILE[7]
 0550 DELETE A6$
 0560 PRINT
 0570 PRINT "<7><7>PATTERN '";A8$;"' HAS BEEN DELETED BECAUSE IT WAS IN
*     COMPLETE."
 0580 GOTO 1860
 0590 CLOSE FILE[4]
 0600 OPEN FILE[4,0],T$,200
 0602 PRINT
 0604 PRINT "HERE ARE THE ALLOWABLE UNITS OF CONCENTRATION:"
 0606 PRINT
 0608 PRINT "      1.   NANOGRAMS PER MICROLITER"
 0610 PRINT "      2.   MICROGRAMS PER LITER"
 0612 PRINT
 0614 ON ERR THEN GOTO 0618
 0616 INPUT "WHICH UNIT DO YOU WANT TO USE? (1 OR 2)  ",X
 0618 ON ERR THEN STOP
 0620 IF X=INT(X) THEN IF X>0 THEN IF X<3 THEN GOTO 0630
 0622 PRINT
 0624 PRINT "<7><7>";X;"IS NOT A VALID UNIT NUMBER."
 0626 GOTO 0602
 0630 PRINT
 0640 FOR I=1 TO 60
 0650   READ FILE[4,3*I-1],V$
 0660   IF EOF(4) THEN GOTO 0770
 0670   IF V$<>"99999" THEN GOTO 0700
 0680   LET A5=9.99999E-07
 0690   GOTO 0750

 1234567891123456789212345678931234567894123456789512345678961234567897
          0          0          0          0          0          0          0
```

PROGRAM LISTING FOR GC02

```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
0700   IF I=1 THEN PRINT "CONCENTRATION OF ";
0710   PRINT  TAB(17);V$;"?"; TAB(28);
0720   ON ERR THEN GOTO 0740
0730   INPUT "",A5
0740   ON ERR THEN STOP
0741   IF A5>0 THEN GOTO 0745
0742   PRINT "<7><7>";A5;"IS NOT A VALID CONCENTRATION VALUE."
0743   GOTO 0700
0745   IF X=1 THEN LET A5=1000*A5
0750   WRITE FILE[7,I],A5
0760 NEXT I
0770 CLOSE FILE[7]
0780 ON ESC THEN GOTO 1830
0790 GOTO 1780
0800 REM   ------------------------------------------------------------
0810 REM          DELETE A CONCENTRATION PATTERN FILE
0820 PRINT
0830 ON ERR THEN GOTO 0850
0840 INPUT "WHAT IS THE NAME OF THE PATTERN TO BE DELETED?  (A, B, C,
*     . . . , OR 7)  ",A8$
0850 ON ERR THEN STOP
0860 LET A7=POS(A9$,A8$,1)
0870 IF A7<>0 THEN GOTO 0910
0880 PRINT
0890 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
0900 GOTO 0820
0910 LET A6$=T$,"000"
0920 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
0930 ON ERR THEN GOTO 0985
0940 DELETE A6$
0950 ON ERR THEN STOP
0960 PRINT
0970 PRINT "PATTERN '";A8$;"' HAS BEEN DELETED."
0980 GOTO 1790
0985 ON ERR THEN STOP
0990 PRINT
1000 PRINT "<7><7>THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1010 PRINT "NO PATTERN HAS BEEN DELETED."
1020 GOTO 1780
1030 REM   ------------------------------------------------------------
1040 REM          DISPLAY A CONCENTRATION PATTERN
1050 PRINT

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC02

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1060 ON ERR THEN GOTO 1080
1070 INPUT "WHAT IS THE NAME OF THE PATTERN TO BE DISPLAYED?  (A, B, C
*     , . . . , OR Z)  ",A8$
1080 ON ERR THEN STOP
1090 LET A7=POS(A9$,A8$,1)
1100 IF A7<>0 THEN GOTO 1140
1110 PRINT
1120 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
1130 GOTO 1050
1140 LET A6$=T$,"000"
1150 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
1160 ON ERR THEN GOTO 1180
1170 RENAME A6$,A6$
1180 ON ERR THEN STOP
1190 IF SYS(7)=-9 THEN GOTO 1230
1200 PRINT
1210 PRINT "<7><7>THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1220 GOTO 1050
1230 ON ERR THEN GOTO 1270
1240 OPEN FILE[7,0],A6$,4
1250 ON ERR THEN STOP
1260 GOTO 1300
1270 ON ERR THEN STOP
1280 DELAY =1
1290 GOTO 1230
1300 CLOSE FILE[4]
1310 OPEN FILE[4,0],T$,200
1320 PRINT
1330 PRINT
1340 PAGE =74
1350 PRINT  TAB(9);"C-O-N-C-E-N-T-R-A-T-I-O-N   P-A-T-T-E-R-N   R-E-P-
*    O-R-T"
1360 PRINT "CONCENTRATION PATTERN:  ";A8$; TAB(53);"METHOD NUMBER:  ";
*    T$[3,6]
1370 PRINT
1380 PRINT "     IDENTIFIER     CONCENTRATION"
1390 PRINT "     ----------     -------------"
1400 FOR I=1 TO 60
1410   READ FILE[4,3*I-1],V$
1420   IF EOF(4) THEN GOTO 1470
1430   IF V$="99999" THEN GOTO 1460
1440   READ FILE[7,I],A5

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
123456789112345678921234567893123456789412345678951234567896123456789 7
        0         0         0         0         0         0         0
1450   PRINT USING "       ########         ####.###",V$,A5
1460 NEXT I
1470 PRINT
1480 PRINT
1490 CLOSE FILE[7]
1500 GOTO 1780
1510 REM    --------------------------------------------------------
1520 REM           LIST EXTANT CONCENTRATION PATTERN FILES
1530 PRINT
1540 PRINT
1550 PRINT  TAB(8);"C-O-N-C-E-N-T-R-A-T-I-O-N  P-A-T-T-E-R-N  L-I-S-
*      T"
1560 PAGE =72
1570 PRINT "CONCENTRATION PATTERNS FOR METHOD ";T$[3,6];":  ";
1580 LET A6$=T$,"000"
1590 LET I2=0
1600 FOR I=1 TO 26
1610   LET A6$[10-LEN(STR$(I)),9]=STR$(I)
1620   ON ERR THEN GOTO 1640
1630   RENAME A6$,A6$
1640   ON ERR THEN STOP
1650   IF SYS(7)<>-9 THEN GOTO 1720
1660   LET I2=I2+1
1670   IF I2<>1 THEN PRINT ", ";
1680   IF I2<>11 THEN GOTO 1710
1690   PRINT
1700   PRINT "     ";
1710   PRINT A9$[I,I];
1720 NEXT I
1730 IF I2=0 THEN PRINT "NONE"
1740 PRINT
1750 PRINT
1760 REM    --------------------------------------------------------
1770 REM           WRAP-UP PROCEDURE
1780 PRINT
1790 ON ERR THEN GOTO 1810
1800 INPUT "DO YOU WANT TO DEAL FURTHER WITH ANY CONCENTRATION PATTERN
*      ?  (Y OR N)  ",X$
1810 ON ERR THEN STOP
1820 IF X$[1,1]="Y" THEN GOTO 0150
1830 ON ERR THEN GOTO 1850
1840 CLOSE FILE[7]

123456789112345678921234567893123456789412345678951234567896123456789 7
        0         0         0         0         0         0         0
```

```
123456789112345678921234567893123456789412345678951234567896123456789 7
        0         0         0         0         0         0         0
1850 ON ERR THEN STOP
1860 NOESC
1870 CHAIN "GC00"

123456789112345678921234567893123456789412345678951234567896123456789 7
        0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE  7
                        SYMBOL TABLE FOR GC02

SYMBOL   REFERENCES
------  -------------------------------------------------------------

 0150   0290  1820
 0250   0230
 0300   0260
 0330   0300  0410  0500
 0360   0340
 0420   0380
 0460   0440
 0510   0470
 0540   0520
 0590   0530
 0602   0626
 0618   0614
 0630   0620
 0700   0670  0743
 0740   0720
 0745   0741
 0750   0690
 0770   0660
 0820   0300  0900
 0850   0830
 0910   0870
 0985   0930
 1050   0300  1130  1220
 1080   1060
 1140   1100
 1180   1160
 1230   1190  1290
 1270   1230
 1300   1260
 1460   1430
 1470   1420
 1530   0300
 1640   1620
 1710   1680
 1720   1650
 1780   0790  0980  1020  1500
 1810   1790
 1830   0080  0780
 1850   1830
 1860   0580
 A5     0680  0730  0741  0742  0745  0750  1440  1450
 A6$    0100  0420  0430  0450  0510  0550  0910  0920  0940  1140
        1150  1170  1240  1580  1610  1630
 A7     0370  0380  0430  0860  0870  0920  1090  1100  1150
 A8$    0100  0350  0370  0400  0490  0570  0840  0860  0890  0970
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE  8
                        SYMBOL TABLE FOR GC02

SYMBOL   REFERENCES
------  -------------------------------------------------------------

        1000  1070  1090  1120  1210  1360
 A9$    0100  0110  0370  0860  1090  1710
 FL#4   0120  0590  0600  0650  1300  1310  1410
 FL#7   0510  0540  0750  0770  1240  1440  1490  1840
 I      0640  0650  0700  0750  0760  1400  1410  1440  1460  1600
        1610  1710  1720
 I2     1590  1660  1670  1680  1730
 T$     0100  0120  0160  0210  0420  0490  0600  0910  1140  1310
        1360  1570  1580
 V$     0100  0650  0670  0710  1410  1430  1450
 X      0240  0260  0280  0300  0616  0620  0624  0745
 X$     0100  1800  1820
```

SECTION 5

PROGRAM GC03 - INTERNAL STANDARDS CALIBRATION

The internal standards calibration method is a planned future enhancement of the GCAS, but it has not been implemented in Version I.

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                          PROGRAM LISTING FOR GC03

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                  +
 0030 REM   +   PROGRAM GC03, INTERNAL STANDARDS CALIBRATION          +
 0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 10, 1979              +
 0045 REM   +   MOST RECENT REVISION:  MARCH 21, 1979                 +
 0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0060 REM
 0070 ESC
 0080 ON ESC THEN GOTO 0120
 0090 PRINT
 0110 PRINT "<7><7>INTERNAL STANDARDS CALIBRATION IS NOT OPERATIONAL AT
*      THIS TIME."
 0120 NOESC
 0130 CHAIN "GC00"




 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                          SYMBOL TABLE FOR GC03

SYMBOL    REFERENCES
------ ---------------------------------------------------------------
 0120  0080
```

SECTION 6

PROGRAM GC04 - PURGE AND TRAP CALIBRATION

GC04 is the program which performs external standards calibration for the purge and trap method. It is entered by chaining from the master control program, GC00, and it chains back to that program when it has been completed or when the escape key is pressed.

The first task of GC04 is to flag the compounds to be calibrated. Array F is a one-dimensional array of flags, as shown in Figure 5. The n^{th} identifier in array F corresponds to the n^{th} identifier in the method file. A "1" in array F indicates that the corresponding identifier is to be calibrated; a zero implies the opposite. The user is asked if all of the compounds are to be calibrated. If so, all of the flags in array F are set to 1. If not all of the identifiers are to be calibrated, the user is asked about each identifier separately, and only the appropriate positions in array F are set to 1.

Next, GC04 asks for the injection ID for a standard, The program checks whether the ID is reasonable and whether the data file exists. It then opens the injection data file and checks the data file useability flag in the first record to see if the data file can be used. It also looks for any error messages in the injection data file and displays them in case they are important to the user.

GC04 then asks the user for the concentration pattern and opens the concentration pattern file. For each flagged identifier, the program searches the injection data file for the peak area and the concentration pattern file for the prepared concentrations. These data elements are placed in the array G, as shown in Figure 5. Each row of array G contains calibration data corresponding to one identifier. Odd numbered columns contain prepared concentrations, and even numbered columns contain peak areas. If the injection data file does not have a peak area for one of the identifiers, the program refuses to use that data file and asks for another. The injection ID for each good data file is concatenated to the superstring I$.

The program continues to ask for more calibration standards until the user types "END" or until the limit of 15 is reached. Then it gives the user the choice of linear regression, quadratic regression, linear interpolation, and linear regression forced through the origin. The program requires at least three standards for linear regression, since three standards are necessary to confirm that the curve is linear. Similarly, at least four standards are required for quadratic regression, since four are necessary to confirm that the curve is parabolic.

The program then branches to one of three curve fitting routines. If the user has selected linear or quadratic regression, the program branches to the normal regression routine. This least squares regression algorithm is documented in great detail in Statistical Methods for Business Decisions by Charles Clark and Lawrence Schkade (South-Western Publishing Company, Cincinnati, Ohio, 1969).

If the user has selected linear interpolation, the program simply puts the calibration standards into ascending order by peak area and writes them into the method file. Array G2, shown in Figure 5, is used to hold one row of array G simply so that it can be placed into the method file by a MAT WRITE FILE statement.

If the user has selected linear regression forced through the origin, the program calculates the equation of a line in the form y=bx, where b is determined by the formula:

$$b = \frac{\sum(\text{Signal} \bullet \text{Concentration})}{\sum(\text{Signal}^2)}$$

For all three types of curve fitting, this program also calculates a "fitting error" which is actually a percent, relative, standard error of estimate, calculated by the formula:

$$\text{Fitting Error} = \frac{100\sqrt{\dfrac{\sum(\text{Known Conc. - Calculated Conc.})^2}{\text{Number of Standards - 2}}}}{\text{Mean Concentration}}$$

When the regression calculations are complete, the calibration data items are written into the method file, and the program chains back to GC00.

TABLE 4. SYMBOL DEFINITIONS FOR PROGRAM GC04.

A6$	the name of a concentration pattern file
A7	the position of A8$ in A9$
A8$	the name of a concentration pattern
A9$	the alphabet
A()	an array used in regression calculations
B	the retention time of a compound
C	the peak area of a compound
D	a holding variable used in a sorting process
D2	a holding variable used in a sorting process
D2$	the injection ID number
D3	a holding variable used in a sorting process
D3$	the name of the data file
D4$	the date of calibration
F	the number of identifiers in the method
F()	the array of flags used to indicate which identifiers are to be calibrated
G$	an identifier read from the data file
G2()	an array consisiting of one row from array G
G()	the array of calibration information (concentrations and peak areas)
H$	the peak type
I	the control variable for several loops
I$	the superstring of injection IDs for the calibration standards

TABLE 4. (continued)

I2$	the superstring of injection IDs in order for linear interpolation purposes
I2	the control variable for several loops
I3	the control variable for several loops
I4	the control variable for several loops
I5	a counter for the number of calibration standards
I6	the control variable for several loops
J	the data file useability flag
J3	the fitting error
J4	the calculated concentration of a standard
J5	the sum of the squares of the differences between the prepared and calculated concentrations of standards
J6	the sum of the concentrations of the standards
J7	used in calculating linear regression forced through the origin
J8	used in calculating linear regression forced through the origin
J9	used in calculating linear regression forced through the origin
P9	the record number of the first record in a data file which describes a peak
R2	the coefficient of the linear term of a regression equation in a linear regression forced through the origin
R()	an array used in regression calculations
T	the method number
T$	the name of the method file
T()	an array used in regression calculations
V$	an identifier from a method file
VO$	an error message from the data file
X	the user's answer to a multiple choice question

TABLE 4 (continued)

X$	the user's answer to a Y or N question
Z3	a variable used in regression calculations

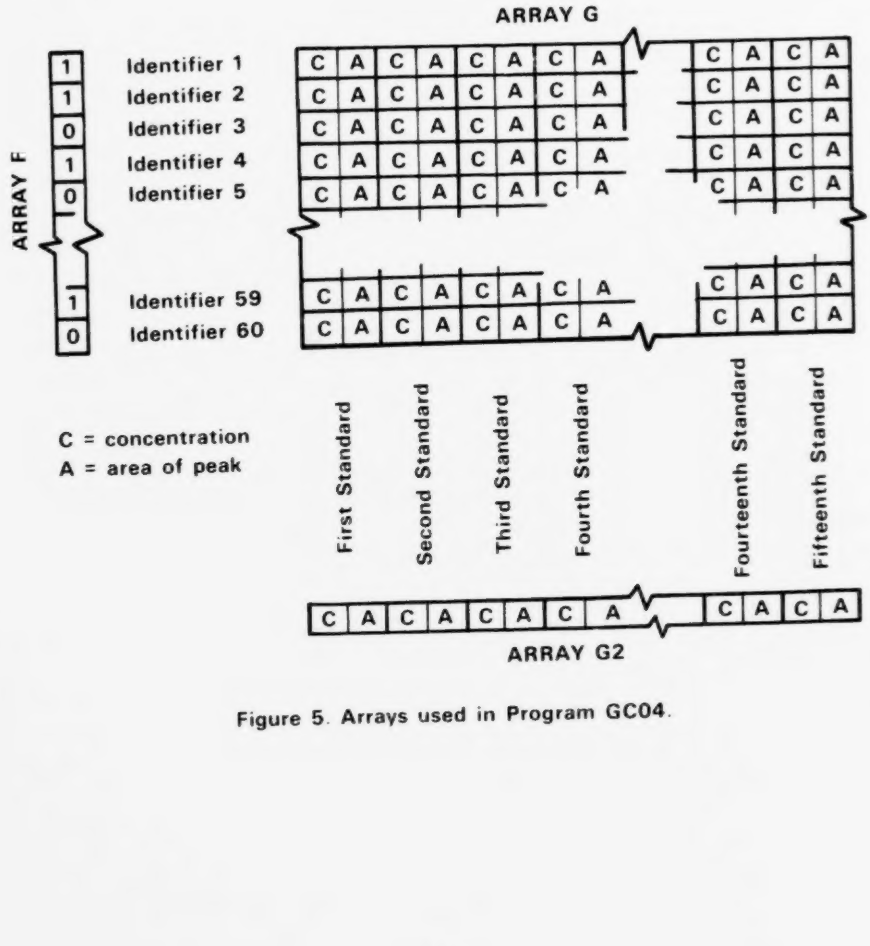

ARRAY G
ARRAY F
1
1
0
1
0
1
0
Identifier 1
Identifier 2
Identifier 3
Identifier 4
Identifier 5
Identifier 59
Identifier 60
C A C A C A C A
C A C A
C = concentration
A = area of peak
First Standard
Second Standard
Third Standard
Fourth Standard
Fourteenth Standard
Fifteenth Standard
ARRAY G2

Figure 5. Arrays used in Program GC04.

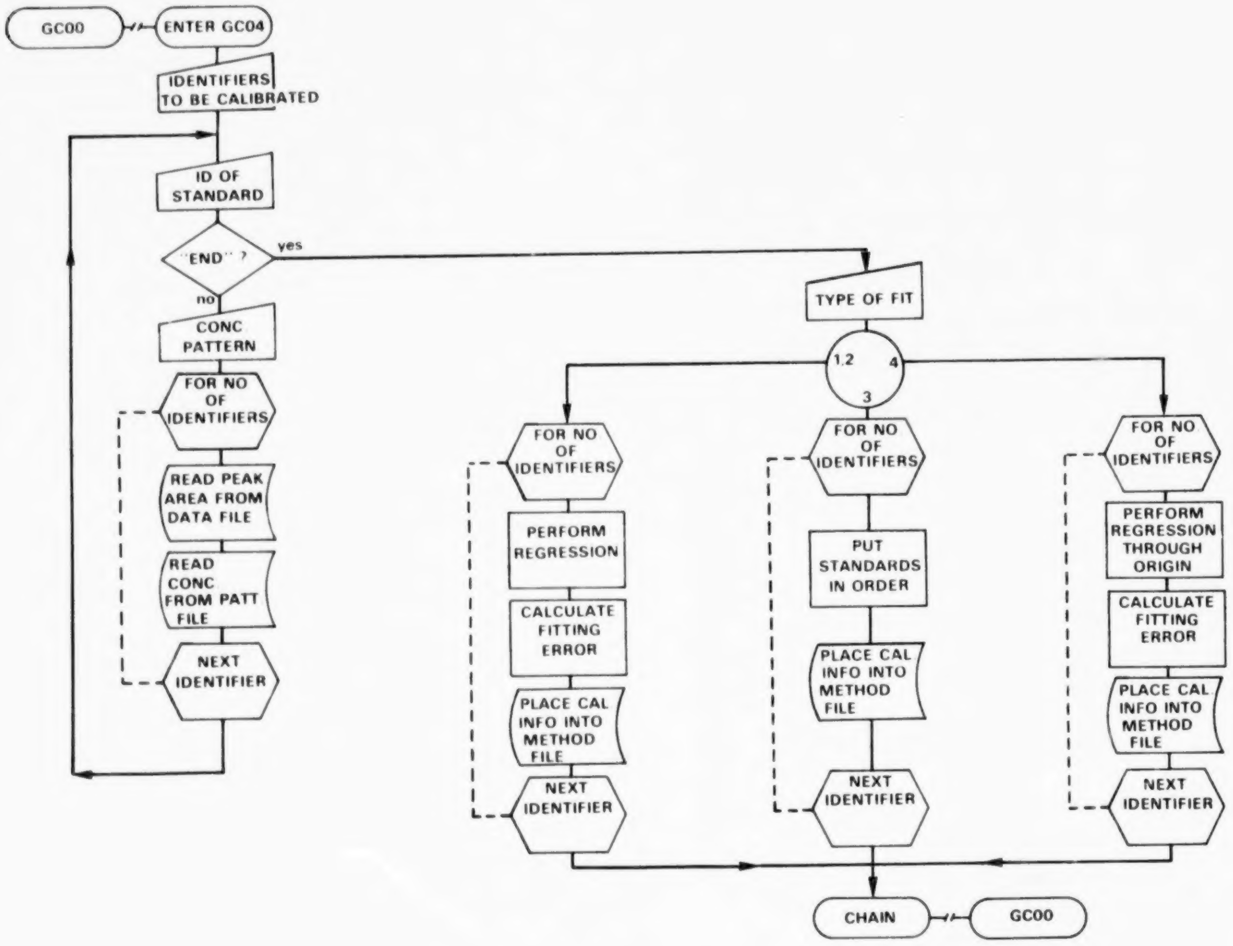

GC00
ENTER GC04
IDENTIFIERS TO BE CALIBRATED
ID OF STANDARD
"END"?
yes
no
CONC PATTERN
FOR NO OF IDENTIFIERS
READ PEAK AREA FROM DATA FILE
READ CONC FROM PATT FILE
NEXT IDENTIFIER
TYPE OF FIT
1,2
3
4
FOR NO OF IDENTIFIERS
PERFORM REGRESSION
CALCULATE FITTING ERROR
PLACE CAL INFO INTO METHOD FILE
NEXT IDENTIFIER
FOR NO OF IDENTIFIERS
PUT STANDARDS IN ORDER
PLACE CAL INFO INTO METHOD FILE
NEXT IDENTIFIER
FOR NO OF IDENTIFIERS
PERFORM REGRESSION THROUGH ORIGIN
CALCULATE FITTING ERROR
PLACE CAL INFO INTO METHOD FILE
NEXT IDENTIFIER
CHAIN
GC00

Figure 6. Flowchart of Program GC04.

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  1
                     PROGRAM LISTING FOR GC04

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC04, EXTERNAL STANDARDS CALIRRATION, P&T       +
0040 REM   +   BY:  J. KOPKE (SWORCC), FEBRUARY 7, 1979                +
0045 REM   +   MOST RECENT REVISION:  APRIL 17, 1979                   +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 3000
0090 DIM A[5],R[3,4],T[4],V0$[20]
0100 DIM F[60],G[60,30],I$[160],T$[6],X$[3],V$[8],D2$[8],D3$[10],D4$[8
*     ],G$[8],H$[2],G2[30],I2$[160]
0105 DIM A9$[26],A8$[1],A6$[9]
0106 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
0110 MAT G=ZER
0120 MAT F=ZER
0130 REM  ------------------------------------------------------------
0140 REM          COUNT NUMRER OF IDENTIFIERS IN METHOD FILE
0150 LET F=0
0160 READ FILE[4,1],T$
0165 CLOSE FILE[4]
0166 OPEN FILE[4,0],T$,200
0170 READ FILE[4,3*(F+1)-1],V$
0180 IF EOF(4) THEN GOTO 0230
0190 LET F=F+1
0200 GOTO 0170
0210 REM  ------------------------------------------------------------
0220 REM          FLAG THE IDENTIFIERS TO BE CALIBRATED
0230 PRINT
0235 PRINT "DO YOU WANT TO CALIBRATE ALL IDENTIFIERS OF METHOD ";T$[3,
*     6];
0237 ON ERR THEN GOTO 0242
0240 INPUT " AT ONCE?  (Y OR N)  ",X$
0242 ON ERR THEN STOP
0250 IF X$[1,1]<>"Y" THEN GOTO 0300
0260 FOR I=1 TO F
0270   LET F[I]=1
0280 NEXT I
0290 GOTO 0410
0300 PRINT
0310 PRINT "DO YOU WANT TO CALIBRATE ";
0320 FOR I=1 TO F

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  2
                     PROGRAM LISTING FOR GC04

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0330   READ FILE[4,3*I-1],V$
0340   IF V$="99999" THEN GOTO 0380
0350   PRINT  TAB(25);V$;"?"; TAB(37);"  (Y OR N)";
0355   ON ERR THEN GOTO 0365
0360   INPUT "  ",X$
0365   ON ERR THEN STOP
0370   IF X$[1,1]="Y" THEN LET F[I]=1
0380 NEXT I
0390 REM  ------------------------------------------------------------
0400 REM          PRINT INSTRUCTIONS FOR ENTERING DATA
0410 PRINT
0420 PRINT "ENTER THE FOLLOWING CALIBRATION INFORMATION."
0440 PRINT "TYPE 'END' AS AN INJECTION ID TO TERMINATE THE LIST."
0450 LET I5=0
0460 REM  ------------------------------------------------------------
0470 REM          OPEN SELECTED DATA FILE
0480 LET I5=I5+1
0490 IF I5<16 THEN GOTO 0540
0500 PRINT
0510 PRINT "<7><7>YOU HAVE USED FIFTEEN CALIBRATION STANDARDS, WHICH I
*     S THE LIMIT"
0520 PRINT "     FOR THIS PROGRAM."
0530 GOTO 1230
0540 PRINT
0545 ON ERR THEN GOTO 0555
0550 INPUT "INJECTION ID FOR CALIBRATION STANDARD?  ",D2$
0555 ON ERR THEN STOP
0560 IF D2$="END" THEN GOTO 1230
0570 IF LEN(D2$)=8 THEN GOTO 0610
0580 PRINT
0590 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID NUMBER."
0600 GOTO 0540
0610 LET D3$="GC",D2$
0620 ON ERR THEN GOTO 0640
0630 RENAME D3$,D3$
0640 ON ERR THEN STOP
0650 IF SYS(7)<>-48 THEN GOTO 0680
0660 DELAY =1
0670 GOTO 0620
0680 IF SYS(7)=-9 THEN GOTO 0720
0690 PRINT
0700 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC04

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0710 GOTO 0540
0720 ON ERR THEN GOTO 0760
0730 OPEN FILE[3,0],D3$,31
0740 ON ERR THEN STOP
0750 GOTO 0810
0760 ON ERR THEN STOP
0770 DELAY =1
0780 GOTO 0720
0790 REM   -----------------------------------------------------------
0800 REM            CHECK DATA FILE USABILITY FLAG
0810 READ FILE[3,1],J
0820 IF J=1 THEN GOTO 0900
0830 PRINT
0840 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*     T DID NOT HAVE A TOTAL AREA."
0850 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*     T WAS IN THE WRONG FORMAT."
0860 CLOSE FILE[3]
0870 GOTO 0540
0880 REM   -----------------------------------------------------------
0890 REM            PRINT ANY ERROR MESSAGES FOUND IN THE DATA FILE
0900 LET P9=2
0910 READ FILE[3,P9],V0$
0920 IF V0$[1,7]<>"MESSAGE" THEN GOTO 1001
0930 PRINT
0940 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
0950 PRINT "     INJECTION ";D2$;":  ";V0$;"."
0960 PRINT
0970 LET P9=P9+1
0980 GOTO 0910
0990 REM   -----------------------------------------------------------
1000 REM            OPEN CONCENTRATION PATTERN FILE
1001 ON ERR THEN GOTO 1003
1002 INPUT "     CONCENTRATION PATTERN FOR STANDARD?  ",A8$
1003 ON ERR THEN STOP
1004 LET A7=POS(A9$,A8$,1)
1005 IF A7<>0 THEN GOTO 1008
1006 PRINT "<7><7>     '";A8$;"' IS NOT A VALID LETTER."
1007 GOTO 1001
1008 LET A6$=T$,"000"
1009 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
1010 ON ERR THEN GOTO 1012

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC04

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1011 RENAME A6$,A6$
1012 ON ERR THEN STOP
1013 IF SYS(7)=-9 THEN GOTO 1016
1014 PRINT "<7><7>     THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1015 GOTO 1001
1016 ON ERR THEN GOTO 1020
1017 OPEN FILE[7,0],A6$,4
1018 ON ERR THEN STOP
1019 GOTO 1026
1020 ON ERR THEN STOP
1021 DELAY =1
1022 GOTO 1016
1024 REM   -----------------------------------------------------------
1025 REM            GATHER CALIBRATION DATA
1026 LET P9=P9+2
1027 FOR I=1 TO F
1030   IF F[I]<>1 THEN GOTO 1190
1040   READ FILE[4,3*I-1],V$
1041   IF V$<>"99999" THEN GOTO 1060
1042   LET F[I]=0
1043   GOTO 1190
1060   READ FILE[7,I],G[I,2*I5-1]
1070   LET I2=P9
1080   READ FILE[3,I2],G$,H$,B,C
1090   IF EOF(3) THEN GOTO 1130
1100   IF G$=V$ THEN IF C<>-9999 THEN GOTO 1180
1110   LET I2=I2+1
1120   GOTO 1080
1130   PRINT
1140   PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" DOES NOT INCLUDE
*     AN AREA FOR ";V$;"."
1150   PRINT "THEREFORE, ";D2$;" CANNOT BE USED IN THIS CALIBRATION."
1160   CLOSE FILE[3]
1165   CLOSE FILE[7]
1170   GOTO 0540
1180   LET G[I,2*I5]=C
1190 NEXT I
1200 CLOSE FILE[3]
1201 CLOSE FILE[7]
1210 LET I$=I$,D2$
1220 GOTO 0480
1230 LET I5=I5-1

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                        PAGE  5
                           PROGRAM LISTING FOR GC04

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1240 IF I5>0 THEN GOTO 1310
1260 PRINT
1270 PRINT "<7><7>BECAUSE NO STANDARDS WERE PROVIDED, NO CALIBRATION H
*    AS BEEN DONE."
1280 GOTO 3000       -----------------------------------------------------
1290 REM    ----------------------------------------------------------
1300 REM            CREATE DATE OF CALIBRATION
1310 LET D4$="00/00/00"
1320 LET D4$[3-LEN(STR$(SYS(2))),2]=STR$(SYS(2))
1330 LET D4$[6-LEN(STR$(SYS(1))),5]=STR$(SYS(1))
1340 LET D4$[9-LEN(STR$(SYS(3)-1900)),8]=STR$(SYS(3)-1900)
1350 REM    ----------------------------------------------------------
1360 REM            SELECT TYPE OF FIT
1370 PRINT
1380 PRINT "HERE ARE THE TYPES OF CALIBRATION CURVE FITTING:"
1390 PRINT
1400 PRINT "     1.  LINEAR REGRESSION"
1410 PRINT "     2.  QUADRATIC REGRESSION"
1420 PRINT "     3.  LINEAR INTERPOLATION EXTENDED TO THE ORIGIN"
1430 PRINT "     4.  LINEAR REGRESSION FORCED THROUGH THE ORIGIN"
1440 PRINT
1445 ON ERR THEN GOTO 1455
1450 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
1455 ON ERR THEN STOP
1460 IF X=1 THEN IF I5>2 THEN GOTO 1500
1465 IF X=2 THEN IF I5>3 THEN GOTO 1500
1470 IF X=3 THEN GOTO 1500
1475 IF X=4 THEN IF I5>2 THEN GOTO 1500
1480 PRINT "<7><7>YOU HAVE NOT USED ENOUGH STANDARDS FOR THIS FIT."
1490 GOTO 1370
1500 ON X THEN GOTO 1890, 1890, 1560, 2650
1510 PRINT
1520 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
1530 GOTO 1370       -----------------------------------------------------
1540 REM    ----------------------------------------------------------
1550 REM            LINEAR INTERPOLATION
1560 FOR I=1 TO F
1570   IF F[I]<>1 THEN GOTO 1830
1580   REM    ----------------------------------
1590   REM      COPY STANDARDS TO SMALLER ARRAY
1600   FOR I2=1 TO 30
1610     LET G2[I2]=G[I,I2]

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                        PAGE  6
                           PROGRAM LISTING FOR GC04

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1620     NEXT I2
1630     REM    ------------------------------------
1640     REM      PUT STANDARDS IN ORDER BY AREA
1645     LET I2$=I$
1650     FOR I3=I5-1 TO 1 STEP -1
1660       FOR I2=1 TO I3
1670         IF G2[2*I2]<G2[2*(I2+1)] THEN GOTO 1770
1680         LET D2=G2[2*I2-1]
1690         LET D3=G2[2*I2]
1700         LET D2$=I2$[8*I2-7,8*I2]
1710         LET G2[2*I2-1]=G2[2*I2+1]
1720         LET G2[2*I2]=G2[2*I2+2]
1730         LET I2$[8*I2-7,8*I2]=I2$[8*(I2+1)-7,8*(I2+1)]
1740         LET G2[2*I2+1]=D2
1750         LET G2[2*I2+2]=D3
1760         LET I2$[8*(I2+1)-7,8*(I2+1)]=D2$
1770       NEXT I2
1780     NEXT I3
1790     REM    ------------------------------------
1800     REM      PUT STANDARDS INTO METHOD FILE
1810     MAT WRITE FILE[4,3*I+1],G2
1820     WRITE FILE[4,3*I],D4$,I2$,X,99999,99999,99999,0
1830 NEXT I
1840 PRINT
1850 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
1860 GOTO 3000   ---------------------------------------------------------
1870 REM    ----------------------------------------------------------
1880 REM         NORMAL FIRST AND SECOND DEGREE REGESSION
1890 FOR I=1 TO F
1900   IF F[I]<>1 THEN GOTO 2590
1910   REM    ------------------------------------
1920   REM      PERFORM REGRESSION
1930   MAT R=ZER
1940   MAT T=ZER
1950   MAT A=ZER
1960   LET A[1]=I5
1970   FOR I2=1 TO I5
1980     FOR I3=2 TO 2*X+1
1990       LET A[I3]=A[I3]+G[I,I2*2]^(I3-1)
2000     NEXT I3
2010     FOR I3=1 TO X+1
2020       LET R[I3,X+2]=T[I3]+G[I,I2*2-1]*G[I,I2*2]^(I3-1)

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
2030        LET T[I3]=T[I3]+G[I,I2*2-1]*G[I,I2*2]^(I3-1)
2040      NEXT I3
2050      LET T[X+2]=T[X+2]+G[I,I2*2-1]^2
2060    NEXT I2
2070    FOR I2=1 TO X+1
2080      FOR I3=1 TO X+1
2090        LET R[I2,I3]=A[I2+I3-1]
2100      NEXT I3
2110    NEXT I2
2120    FOR I2=1 TO X+1
2130      FOR I3=I2 TO X+1
2140        IF R[I3,I2]<>0 THEN GOTO 2210
2150      NEXT I3
2160      READ FILE[4,3*I-1],V$
2170      PRINT
2180      PRINT "<7><7>THERE IS NO UNIQUE SOLUTION FOR THE CALIBRATION
*   EQUATION FOR ";V$;"."
2190      PRINT "THEREFORE, ";V$;" HAS NOT BEEN CALIBRATED."
2200      GOTO 2590
2210      FOR I4=1 TO X+1
2220        LET D=R[I2,I4]
2230        LET R[I2,I4]=R[I3,I4]
2240        LET R[I3,I4]=D
2250      NEXT I4
2260      LET Z3=1/R[I2,I2]
2270      FOR I4=1 TO X+2
2280        LET R[I2,I4]=Z3*R[I2,I4]
2290      NEXT I4
2300      FOR I4=1 TO X+1
2310        IF I4=I2 THEN GOTO 2360
2320        LET Z3=-1*R[I4,I2]
2330        FOR I6=1 TO X+2
2340          LET R[I4,I6]=R[I4,I6]+Z3*R[I2,I6]
2350        NEXT I6
2360      NEXT I4
2370    NEXT I2
2380    REM    ------------------------------------
2390    REM      CALCULATE FITTING ERROR
2400    LET J5=0
2410    LET J6=0
2420    FOR I2=1 TO I5
2430      LET J4=R[1,X+2]+G[I,I2*2]*R[2,X+2]

12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
```

```
12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
2440        IF X=2 THEN LET J4=J4+R[3,X+2]*G[I,I2*2]^2
2450        LET J5=J5+(G[I,I2*2-1]-J4)^2
2460        LET J6=J6+G[I,I2*2-1]
2470      NEXT I2
2480      LET J3=SQR(J5/(I5-2))/(J6/I5)
2490      LET J3=J3*100
2500      REM    ------------------------------------
2510      REM      COPY STANDARDS INTO SMALLER ARRAY
2520      FOR I2=1 TO 30
2530        LET G2[I2]=G[I,I2]
2540      NEXT I2
2550      REM    ------------------------------------
2560      REM      PUT STANDARDS INTO METHOD FILE
2570      MAT WRITE FILE[4,3*I+1],G2
2580      WRITE FILE[4,3*I],D4$,I$,X,R[1,X+2],R[2,X+2].R[3,X+2],J3
2590    NEXT I
2600    PRINT
2610    PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
2620    GOTO 3000
2630    REM    ----------------------------------------------------------
2640    REM            LINEAR REGRESSION FORCED THROUGH THE ORIGIN
2650    FOR I=1 TO F
2660      LET J7=0
2670      LET J8=0
2680      LET J9=0
2690      IF F[I]<>1 THEN GOTO 2950
2700      FOR I2=1 TO I5
2710        LET J7=J7+G[I,I2*2-1]*G[I,I2*2]
2720        LET J8=J8+G[I,I2*2]^2
2730        LET J9=J9+G[I,I2*2-1]
2740      NEXT I2
2750      LET R2=J7/J8
2760      REM    ------------------------------------
2770      REM      CALCULATE FITTING ERROR
2780      LET J5=0
2790      LET J6=0
2800      FOR I2=1 TO I5
2810        LET J5=J5+(G[I,I2*2-1]-G[I,I2*2]*R2)^2
2820        LET J6=J6+G[I,I2*2-1]
2830      NEXT I2
2840      LET J3=SQR(J5/(I5-2))/(J6/I5)
2850      LET J3=J3*100

12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  9
                         PROGRAM LISTING FOR GC04

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
2860   REM   -----------------------------------------
2870   REM     COPY STANDARDS INTO SMALLER ARRAY
2880   FOR I2=1 TO 30
2890     LET G2[I2]=G[I,I2]
2900   NEXT I2
2910   REM   -----------------------------------------
2920   REM     PUT DATA INTO METHOD FILE
2930   MAT WRITE FILE[4,3*I+1],G2
2940   WRITE FILE[4,3*I],D4$,I$,X,0,R2,0,J3
2950 NEXT I
2960 PRINT
2970 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
2980 REM   -------------------------------------------------------
2990 REM             RETURN TO MASTER CONTROL
3000 ON ERR THEN GOTO 3020
3010 CLOSE FILE[3]
3020 ON ERR THEN GOTO 3040
3030 CLOSE FILE[7]
3040 ON ERR THEN STOP
3050 NOESC
3060 CHAIN "GC00"

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE 10
                          SYMBOL TABLE FOR GC04
SYMBOL   REFERENCES
------   ------------------------------------------------------------
0170  0200
0230  0180
0242  0237
0300  0250
0365  0355
0380  0340
0410  0290
0480  1220
0540  0490  0600  0710  0870  1170
0555  0545
0610  0570
0620  0670
0640  0620
0680  0650
0720  0680  0780
0760  0720
0810  0750
0900  0820
0910  0980
1001  0920  1007  1015
1003  1001
1008  1005
1012  1010
1016  1013  1022
1020  1016
1026  1019
1060  1041
1080  1120
1130  1090
1180  1100
1190  1030  1043
1230  0530  0560
1310  1240
1370  1490  1530
1455  1445
1500  1460  1465  1470  1475
1560  1500
1770  1670
1830  1570
1890  1500
2210  2140
2360  2310
2590  1900  2200
2650  1500
2950  2690
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE 11
                       SYMBOL TABLE FOR GC04

SYMBOL    REFERENCES
------  ---------------------------------------------------------------
 3000   0080  1280  1860  2620
 3020   3000
 3040   3020
 A      1950
 A6$    0105  1008  1009  1011  1017
 A7     1004  1005  1009
 A8$    0105  1002  1004  1006  1014
 A9$    0105  0106  1004
 A[     0090  1960  1990  2090
 B      1080
 C      1080  1100  1180
 D      2220  2240
 D2     1680  1740
 D2$    0100  0550  0560  0570  0590  0610  0700  0840  0850  0950
        1140  1150  1210  1700  1760
 D3     1690  1750
 D3$    0100  0610  0630  0730
 D4$    0100  1310  1320  1330  1340  1820  2580  2940
 F      0120  0150  0170  0190  0260  0320  1027  1560  1890  2650
 FL#3   0730  0810  0860  0910  1080  1160  1200  3010
 FL#4   0160  0165  0166  0170  0330  1040  1810  1820  2160  2570
        2580  2930  2940
 FL#7   1017  1060  1165  1201  3030
 F[     0100  0270  0370  1030  1042  1570  1900  2690
 G      0110
 G$     0100  1080  1100
 G2     1810  2570  2930
 G2[    0100  1610  1670  1680  1690  1710  1720  1740  1750  2530
        2890
 G[     0100  1060  1180  1610  1990  2020  2030  2050  2430  2440
        2450  2460  2530  2710  2720  2730  2810  2820  2890
 H$     0100  1080
 I      0260  0270  0280  0320  0330  0370  0380  1027  1030  1040
        1042  1060  1180  1190  1560  1570  1610  1810  1820  1830
        1890  1900  1990  2020  2030  2050  2160  2430  2440  2450
        2460  2530  2570  2580  2590  2650  2690  2710  2720  2730
        2810  2820  2890  2930  2940  2950
 I$     0100  1210  1645  2580  2940
 I2     1070  1080  1110  1600  1610  1620  1660  1670  1680  1690
        1700  1710  1720  1730  1740  1750  1760  1770  1970  1990
        2020  2030  2050  2060  2070  2090  2110  2120  2130  2140
        2220  2230  2260  2280  2310  2320  2340  2370  2420  2430
        2440  2450  2460  2470  2520  2530  2540  2700  2710  2720
        2730  2740  2800  2810  2820  2830  2880  2890  2900
 I2$    0100  1645  1700  1730  1760  1820
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE 12
                       SYMBOL TABLE FOR GC04

SYMBOL    REFERENCES
------  ---------------------------------------------------------------
 I3     1650  1660  1780  1980  1990  2000  2010  2020  2030  2040
        2080  2090  2100  2130  2140  2150  2230  2240
 I4     2210  2220  2230  2240  2250  2270  2280  2290  2300  2310
        2320  2340  2360
 I5     0450  0480  0490  1060  1180  1230  1240  1460  1465  1475
        1650  1960  1970  2420  2480  2700  2800  2840
 I6     2330  2340  2350
 J      0810  0820  0840  0850
 J3     2480  2490  2580  2840  2850  2940
 J4     2430  2440  2450
 J5     2400  2450  2480  2780  2810  2940
 J6     2410  2460  2480  2790  2820  2840
 J7     2660  2710  2750
 J8     2670  2720  2750
 J9     2680  2730
 P9     0900  0910  0970  1026  1070
 R      1930
 R2     2750  2810  2940
 R[     0090  2020  2090  2140  2220  2230  2240  2260  2280  2320
        2340  2430  2440  2580
 T      1940
 T$     0100  0160  0166  0235  1008  1850  2610  2970
 T[     0090  2020  2030  2050
 V$     0100  0170  0330  0340  0350  1040  1041  1100  1140  2160
        2180  2190
 V0$    0090  0910  0920  0950
 X      1450  1460  1465  1470  1475  1500  1520  1820  1980  2010
        2020  2050  2070  2080  2120  2130  2210  2270  2300  2330
        2430  2440  2580  2940
 X$     0100  0240  0250  0360  0370
 Z3     2260  2280  2320  2340
```

SECTION 7

PROGRAM GC05 - LIQUID/LIQUID EXTRACTION AND DIRECT AQUEOUS INJECTION CALIBRATION

GC05 is the program which performs calibration for standards prepared by the liquid/liquid extraction and direct aqueous injection methods. It is essentially the same as program GC04. The only difference is that in addition to asking the user for the concentration of each compound, this program also asks for the injection volume of each standard. It then multiplies the prepared concentration (in micrograms per liter) times the injection volume (in microliters) times 1000 to get the mass (in nanograms) of each compound. Calibration is then done on the basis of mass.

One additional symbol is used in GC05. It is Z, the volume of the injection.

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  1
                    PROGRAM LISTING FOR GC05

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                     +
 0030 REM   +   PROGRAM GC05, EXTERNAL STANDARDS CALIBRATION, L/L, DAI+
 0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 19, 1979                   +
 0045 REM   +   MOST RECENT REVISION:  APRIL 17, 1979                    +
 0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0060 REM
 0070 ESC
 0080 ON ESC THEN GOTO 3000
 0090 DIM A[5],R[3,4],T[4],V0$[20]
 0100 DIM F[60],G[60,30],I$[160],T$[6],X$[3],V$[8],D2$[8],D3$[10],D4$[8
*     ],G$[8],H$[2],G2[30],I2$[160]
 0105 DIM A9$[26],A8$[1],A6$[9]
 0106 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
 0110 MAT G=ZER
 0120 MAT F=ZER
 0130 REM   ------------------------------------------------------------
 0140 REM           COUNT NUMBER OF IDENTIFIERS IN METHOD FILE
 0150 LET F=0
 0160 READ FILE[4,1],T$
 0165 CLOSE FILE[4]
 0166 OPEN FILE[4,0],T$,200
 0170 READ FILE[4,3*(F+1)-1],V$
 0180 IF EOF(4) THEN GOTO 0230
 0190 LET F=F+1
 0200 GOTO 0170
 0210 REM   ------------------------------------------------------------
 0220 REM           FLAG THE IDENTIFIERS TO BE CALIBRATED
 0230 PRINT
 0235 PRINT "DO YOU WANT TO CALIBRATE ALL IDENTIFIERS OF METHOD ";T$[3,
*     6];
 0237 ON ERR THEN GOTO 0242
 0240 INPUT " AT ONCE?  (Y OR N)  ",X$
 0242 ON ERR THEN STOP
 0250 IF X$[1,1]<>"Y" THEN GOTO 0300
 0260 FOR I=1 TO F
 0270   LET F[I]=1
 0280 NEXT I
 0290 GOTO 0410
 0300 PRINT
 0310 PRINT "DO YOU WANT TO CALIBRATE ";
 0320 FOR I=1 TO F

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  2
                    PROGRAM LISTING FOR GC05

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0330   READ FILE[4,3*I-1],V$
0340   IF V$="99999" THEN GOTO 0380
0350   PRINT  TAB(25);V$;"?"; TAB(37);"  (Y OR N)";
0355   ON ERR THEN GOTO 0365
0360   INPUT "  ",X$
0365   ON ERR THEN STOP
0370   IF X$[1,1]="Y" THEN LET F[I]=1
0380 NEXT I
0390 REM   ------------------------------------------------------------
0400 REM          PRINT INSTRUCTIONS FOR ENTERING DATA
0410 PRINT
0420 PRINT "ENTER THE FOLLOWING CALIBRATION INFORMATION."
0440 PRINT "TYPE 'END' AS AN INJECTION ID TO TERMINATE THE LIST."
0450 LET I5=0
0460 REM   ------------------------------------------------------------
0470 REM          OPEN SELECTED DATA FILE
0480 LET I5=I5+1
0490 IF I5<16 THEN GOTO 0540
0500 PRINT
0510 PRINT "<7><7>YOU HAVE USED FIFTEEN CALIBRATION STANDARDS, WHICH I
*    S THE LIMIT"
0520 PRINT "     FOR THIS PROGRAM."
0530 GOTO 1230
0540 PRINT
0545 ON ERR THEN GOTO 0555
0550 INPUT "INJECTION ID FOR CALIBRATION STANDARD?  ",D2$
0555 ON ERR THEN STOP
0560 IF D2$="END" THEN GOTO 1230
0570 IF LEN(D2$)=8 THEN GOTO 0610
0580 PRINT
0590 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID NUMBER."
0600 GOTO 0540
0610 LET D3$="GC",D2$
0620 ON ERR THEN GOTO 0640
0630 RENAME D3$,D3$
0640 ON ERR THEN STOP
0650 IF SYS(7)<>-48 THEN GOTO 0680
0660 DELAY =1
0670 GOTO 0620
0680 IF SYS(7)=-9 THEN GOTO 0720
0690 PRINT
0700 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/24/1979                                                       PAGE  3
                    PROGRAM LISTING FOR GC05

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
0710 GOTO 0540
0720 ON ERR THEN GOTO 0760
0730 OPEN FILE[3,0],D3$,31
0740 ON ERR THEN STOP
0750 GOTO 0810
0760 ON ERR THEN STOP
0770 DELAY =1
0780 GOTO 0720
0790 REM  -------------------------------------------------------------
0800 REM         CHECK DATA FILE USABILITY FLAG
0810 READ FILE[3,1],J
0820 IF J=1 THEN GOTO 0900
0830 PRINT
0840 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*     T DID NOT HAVE A TOTAL AREA."
0850 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*     T WAS IN THE WRONG FORMAT."
0860 CLOSE FILE[3]
0870 GOTO 0540
0880 REM  -------------------------------------------------------------
0890 REM         PRINT ANY ERROR MESSAGES FOUND IN THE DATA FILE
0900 LET P9=2
0910 READ FILE[3,P9],V0$
0920 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0992
0930 PRINT
0940 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
0950 PRINT "     INJECTION ";D2$;":  ";V0$;"."
0960 PRINT
0970 LET P9=P9+1
0980 GOTO 0910
0990 REM  -------------------------------------------------------------
0991 REM         OPEN CONCENTRATION PATTERN FILE
0992 ON ERR THEN GOTO 0994
0993 INPUT "     CONCENTRATION PATTERN FOR STANDARD?  ",A8$
0994 ON ERR THEN STOP
0995 LET A7=POS(A9$,A8$,1)
0996 IF A7<>0 THEN GOTO 0999
0997 PRINT "<7><7>     '";A8$;"' IS NOT A VALID LETTER."
0998 GOTO 0992
0999 LET A6$=T$,"000"
1000 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
1001 ON ERR THEN GOTO 1003

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/24/1979                                                       PAGE  4
                    PROGRAM LISTING FOR GC05

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
1002 RENAME A6$,A6$
1003 ON ERR THEN STOP
1004 IF SYS(7)=-9 THEN GOTO 1007
1005 PRINT "<7><7>     THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1006 GOTO 0992
1007 ON ERR THEN GOTO 1011
1008 OPEN FILE[7,0],A6$,4
1009 ON ERR THEN STOP
1010 GOTO 1020
1011 ON ERR THEN STOP
1012 DELAY =1
1013 GOTO 1007
1015 REM  -------------------------------------------------------------
1016 REM         GATHER CALIBRATION DATA
1020 ON ERR THEN GOTO 1022
1021 INPUT "     INJECTION VOLUME IN MICROLITERS?  ",Z
1022 ON ERR THEN STOP
1023 LET P9=P9+2
1024 FOR I=1 TO F
1030   IF F[I]<>1 THEN GOTO 1190
1040   READ FILE[4,3*I-1],V$
1041   IF V$<>"99999" THEN GOTO 1060
1042   LET F[I]=0
1043   GOTO 1190
1060   READ FILE[7,I],G[I,2*I5-1]
1065   LET G[I,2*I5-1]=G[I,2*I5-1]*Z*1000
1070   LET I2=P9
1080   READ FILE[3,I2],G$,H$,B,C
1090   IF EOF(3) THEN GOTO 1130
1100   IF G$=V$ THEN IF C<>-9999 THEN GOTO 1180
1110   LET I2=I2+1
1120   GOTO 1080
1130   PRINT
1140   PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" DOES NOT INCLUDE
*     AN AREA FOR ";V$;"."
1150   PRINT "THEREFORE, ";D2$;" CANNOT BE USED IN THIS CALIBRATION."
1160   CLOSE FILE[3]
1165   CLOSE FILE[7]
1170   GOTO 0540
1180   LET G[I,2*I5]=C
1190 NEXT I
1200 CLOSE FILE[3]

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1201 CLOSE FILE[7]
1210 LET I$=I$,D2$
1220 GOTO 0480
1230 LET I5=I5-1
1240 IF I5>0 THEN GOTO 1310
1260 PRINT
1270 PRINT "<7><7>BECAUSE NO STANDARDS WERE PROVIDED, NO CALIBRATION H
*    AS BEEN DONE."
1280 GOTO 3000
1290 REM     -------------------------------------------------------------
1300 REM             CREATE DATE OF CALIBRATION
1310 LET D4$="00/00/00"
1320 LET D4$[3-LEN(STR$(SYS(2))),2]=STR$(SYS(2))
1330 LET D4$[6-LEN(STR$(SYS(1))),5]=STR$(SYS(1))
1340 LET D4$[9-LEN(STR$(SYS(3)-1900)),8]=STR$(SYS(3)-1900)
1350 REM     -------------------------------------------------------------
1360 REM             SELECT TYPE OF FIT
1370 PRINT
1380 PRINT "HERE ARE THE TYPES OF CALIBRATION CURVE FITTING:"
1390 PRINT
1400 PRINT "     1.  LINEAR REGRESSION"
1410 PRINT "     2.  QUADRATIC REGRESSION"
1420 PRINT "     3.  LINEAR INTERPOLATION EXTENDED TO THE ORIGIN"
1430 PRINT "     4.  LINEAR REGRESSION FORCED THROUGH THE ORIGIN"
1440 PRINT
1445 ON ERR THEN GOTO 1455
1450 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
1455 ON ERR THEN STOP
1460 IF X=1 THEN IF I5>2 THEN GOTO 1500
1465 IF X=2 THEN IF I5>3 THEN GOTO 1500
1470 IF X=3 THEN GOTO 1500
1475 IF X=4 THEN IF I5>2 THEN GOTO 1500
1480 PRINT "<7><7>YOU HAVE NOT USED ENOUGH STANDARDS FOR THIS FIT."
1490 GOTO 1370
1500 ON X THEN GOTO 1890, 1890, 1560, 2650
1510 PRINT
1520 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
1530 GOTO 1370
1540 REM     -------------------------------------------------------------
1550 REM             LINEAR INTERPOLATION
1560 FOR I=1 TO F
1570   IF F[I]<>1 THEN GOTO 1830

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1580   REM    ---------------------------------------
1590   REM      COPY STANDARDS TO SMALLER ARRAY
1600   FOR I2=1 TO 30
1610     LET G2[I2]=G[I,I2]
1620   NEXT I2
1630   REM    ---------------------------------------
1640   REM      PUT STANDARDS IN ORDER BY AREA
1645   LET I2$=I$
1650   FOR I3=I5-1 TO 1 STEP -1
1660     FOR I2=1 TO I3
1670       IF G2[2*I2]<G2[2*(I2+1)] THEN GOTO 1770
1680       LET D2=G2[2*I2-1]
1690       LET D3=G2[2*I2]
1700       LET D2$=I2$[8*I2-7,8*I2]
1710       LET G2[2*I2-1]=G2[2*I2+1]
1720       LET G2[2*I2]=G2[2*I2+2]
1730       LET I2$[8*I2-7,8*I2]=I2$[8*(I2+1)-7,8*(I2+1)]
1740       LET G2[2*I2+1]=D2
1750       LET G2[2*I2+2]=D3
1760       LET I2$[8*(I2+1)-7,8*(I2+1)]=D2$
1770     NEXT I2
1780   NEXT I3
1790   REM    ---------------------------------------
1800   REM      PUT STANDARDS INTO METHOD FILE
1810   MAT WRITE FILE[4,3*I+1],G2
1820   WRITE FILE[4,3*I],D4$,I2$,X,99999,99999,99999,0
1830 NEXT I
1840 PRINT
1850 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
1860 GOTO 3000
1870 REM     -------------------------------------------------------------
1880 REM             NORMAL FIRST AND SECOND DEGREE REGESSION
1890 FOR I=1 TO F
1900   IF F[I]<>1 THEN GOTO 2590
1910   REM    ---------------------------------------
1920   REM      PERFORM REGRESSION
1930   MAT R=ZER
1940   MAT T=ZER
1950   MAT A=ZER
1960   LET A[1]=I5
1970   FOR I2=1 TO I5
1980     FOR I3=2 TO 2*X+1

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
 12345678911234567892123456789312345678941234567895123456789612345678970
          0         0         0         0         0         0         0
 1990        LET A[I3]=A[I3]+G[I,I2*2]^(I3-1)
 2000      NEXT I3
 2010      FOR I3=1 TO X+1
 2020        LET R[I3,X+2]=T[I3]+G[I,I2*2-1]*G[I,I2*2]^(I3-1)
 2030        LET T[I3]=T[I3]+G[I,I2*2-1]*G[I,I2*2]^(I3-1)
 2040      NEXT I3
 2050      LET T[X+2]=T[X+2]+G[I,I2*2-1]^2
 2060    NEXT I2
 2070    FOR I2=1 TO X+1
 2080      FOR I3=1 TO X+1
 2090        LET R[I2,I3]=A[I2+I3-1]
 2100      NEXT I3
 2110    NEXT I2
 2120    FOR I2=1 TO X+1
 2130      FOR I3=I2 TO X+1
 2140        IF R[I3,I2]<>0 THEN GOTO 2210
 2150      NEXT I3
 2160      READ FILE[4,3*I-1],V$
 2170      PRINT
 2180      PRINT "<7><7>THERE IS NO UNIQUE SOLUTION FOR THE CALIBRATION
*      EQUATION FOR ";V$;"."
 2190      PRINT "THEREFORE, ";V$;" HAS NOT BEEN CALIBRATED."
 2200      GOTO 2590
 2210      FOR I4=1 TO X+1
 2220        LET D=R[I2,I4]
 2230        LET R[I2,I4]=R[I3,I4]
 2240        LET R[I3,I4]=D
 2250      NEXT I4
 2260      LET Z3=1/R[I2,I2]
 2270      FOR I4=1 TO X+2
 2280        LET R[I2,I4]=Z3*R[I2,I4]
 2290      NEXT I4
 2300      FOR I4=1 TO X+1
 2310        IF I4=I2 THEN GOTO 2360
 2320        LET Z3=-1*R[I4,I2]
 2330        FOR I6=1 TO X+2
 2340          LET R[I4,I6]=R[I4,I6]+Z3*R[I2,I6]
 2350        NEXT I6
 2360      NEXT I4
 2370    NEXT I2
 2380    REM    ------------------------------------
 2390    REM      CALCULATE FITTING ERROR

 12345678911234567892123456789312345678941234567895123456789612345678970
          0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
  2400   LET J5=0
  2410   LET J6=0
  2420   FOR I2=1 TO I5
  2430     LET J4=R[1,X+2]+G[I,I2*2]*R[2,X+2]
  2440     IF X=2 THEN LET J4=J4+R[3,X+2]*G[I,I2*2]^2
  2450     LET J5=J5+(G[I,I2*2-1]-J4)^2
  2460     LET J6=J6+G[I,I2*2-1]
  2470   NEXT I2
  2480   LET J3=SQR(J5/(I5-2))/(J6/I5)
  2490   LET J3=J3*100
  2500   REM    ------------------------------------
  2510   REM      COPY STANDARDS INTO SMALLER ARRAY
  2520   FOR I2=1 TO 30
  2530     LET G2[I2]=G[I,I2]
  2540   NEXT I2
  2550   REM    ------------------------------------
  2560   REM      PUT STANDARDS INTO METHOD FILE
  2570   MAT WRITE FILE[4,3*I+1],G2
  2580   WRITE FILE[4,3*I],D4$,I$,X,R[1,X+2],R[2,X+2],R[3,X+2],J3
  2590 NEXT I
  2600 PRINT
  2610 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
  2620 GOTO 3000
  2630 REM    ---------------------------------------------------------
  2640 REM            LINEAR REGRESSION FORCED THROUGH THE ORIGIN
  2650 FOR I=1 TO F
  2660   LET J7=0
  2670   LET J8=0
  2680   LET J9=0
  2690   IF F[I]<>1 THEN GOTO 2950
  2700   FOR I2=1 TO I5
  2710     LET J7=J7+G[I,I2*2-1]*G[I,I2*2]
  2720     LET J8=J8+G[I,I2*2]^2
  2730     LET J9=J9+G[I,I2*2-1]
  2740   NEXT I2
  2750   LET R2=J7/J8
  2760   REM    ------------------------------------
  2770   REM      CALCULATE FITTING ERROR
  2780   LET J5=0
  2790   LET J6=0
  2800   FOR I2=1 TO I5
  2810     LET J5=J5+(G[I,I2*2-1]-G[I,I2*2]*R2)^2

12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  9
                    PROGRAM LISTING FOR GC05

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
2820     LET J6=J6+G[I,I2*2-1]
2830   NEXT I2
2840   LET J3=SQR(J5/(I5-2))/(J6/I5)
2850   LET J3=J3*100
2860   REM   ---------------------------------------
2870   REM      COPY STANDARDS INTO SMALLER ARRAY
2880   FOR I2=1 TO 30
2890     LET G2[I2]=G[I,I2]
2900   NEXT I2
2910   REM   ---------------------------------------
2920   REM      PUT DATA INTO METHOD FILE
2930   MAT WRITE FILE[4,3*I+1],G2
2940   WRITE FILE[4,3*I],D4$,I$,X,0,R2,0,J3
2950 NEXT I
2960 PRINT
2970 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
2980 REM   ------------------------------------------------------------
2990 REM            RETURN TO MASTER CONTROL
3000 ON ERR THEN GOTO 3020
3010 CLOSE FILE[3]
3020 ON ERR THEN GOTO 3040
3030 CLOSE FILE[7]
3040 ON ERR THEN STOP
3050 NOESC
3060 CHAIN "GC00"











1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE 10
                     SYMBOL TABLE FOR GC05

SYMBOL    REFERENCES
------  ------------------------------------------------------------
 0170  0200
 0230  0180
 0242  0237
 0300  0250
 0365  0355
 0380  0340
 0410  0290
 0480  1220
 0540  0490  0600  0710  0870  1170
 0555  0545
 0610  0570
 0620  0670
 0640  0620
 0680  0650
 0720  0680  0780
 0760  0720
 0810  0750
 0900  0820
 0910  0980
 0992  0920  0998  1006
 0994  0992
 0999  0996
 1003  1001
 1007  1004  1013
 1011  1007
 1020  1010
 1022  1020
 1060  1041
 1080  1120
 1130  1090
 1180  1100
 1190  1030  1043
 1230  0530  0560
 1310  1240
 1370  1490  1530
 1455  1445
 1500  1460  1465  1470  1475
 1560  1500
 1770  1670
 1830  1570
 1890  1500
 2210  2140
 2360  2310
 2590  1900  2200
 2650  1500
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE 11
                      SYMBOL TABLE FOR GC05

SYMBOL   REFERENCES
------ -----------------------------------------------------------------
 2950  2690
 3000  0080  1280  1860  2620
 3020  3000
 3040  3020
 A     1950
 A6$   0105  0999  1000  1002  1008
 A7    0995  0996  1000
 A8$   0105  0993  0995  0997  1005
 A9$   0105  0106  0995
 A[    0090  1960  1990  2090
 B     1080
 C     1080  1100  1180
 D     2220  2240
 D2    1680  1740
 D2$   0100  0550  0560  0570  0590  0610  0700  0840  0850  0950
       1140  1150  1210  1700  1760
 D3    1690  1750
 D3$   0100  0610  0630  0730
 D4$   0100  1310  1320  1330  1340  1820  2580  2940
 F     0120  0150  0170  0190  0260  0320  1024  1560  1890  2650
 FL#3  0730  0810  0860  0910  1080  1160  1200  3010
 FL#4  0160  0165  0166  0170  0330  1040  1810  1820  2160  2570
       2580  2930  2940
 FL#7  1008  1060  1165  1201  3030
 F[    0100  0270  0370  1030  1042  1570  1900  2690
 G     0110
 G$    0100  1080  1100
 G2    1810  2570  2930
 G2[   0100  1610  1670  1680  1690  1710  1720  1740  1750  2530
       2890
 G[    0100  1060  1065  1180  1610  1990  2020  2030  2050  2430
       2440  2450  2460  2530  2710  2720  2730  2810  2820  2890
 H$    0100  1080
 I     0260  0270  0280  0320  0330  0370  0380  1024  1030  1040
       1042  1060  1065  1180  1190  1560  1570  1610  1810  1820
       1830  1890  1900  1990  2020  2030  2050  2160  2430  2440
       2450  2460  2530  2570  2580  2590  2650  2690  2710  2720
       2730  2810  2820  2890  2930  2940  2950
 I$    0100  1210  1645  2580  2940
 I2    1070  1080  1110  1600  1610  1620  1660  1670  1680  1690
       1700  1710  1720  1730  1740  1750  1760  1770  1970  1990
       2020  2030  2050  2060  2070  2090  2110  2120  2130  2140
       2220  2230  2260  2280  2310  2320  2340  2370  2420  2430
       2440  2450  2460  2470  2520  2530  2540  2700  2710  2720
       2730  2740  2800  2810  2820  2830  2880  2890  2900
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE 12
                      SYMBOL TABLE FOR GC05

SYMBOL   REFERENCES
------ -----------------------------------------------------------------
 I2$   0100  1645  1700  1730  1760  1820
 I3    1650  1660  1780  1980  1990  2000  2010  2020  2030  2040
       2080  2090  2100  2130  2140  2150  2230  2240
 I4    2210  2220  2230  2240  2250  2270  2280  2290  2300  2310
       2320  2340  2360
 I5    0450  0480  0490  1060  1065  1180  1230  1240  1460  1465
       1475  1650  1960  1970  2420  2480  2700  2800  2840
 I6    2330  2340  2350
 J     0810  0820  0840  0850
 J3    2480  2490  2580  2840  2850  2940
 J4    2430  2440  2450
 J5    2400  2450  2480  2780  2810  2840
 J6    2410  2460  2480  2790  2820  2840
 J7    2660  2710  2750
 J8    2670  2720  2750
 J9    2680  2730
 P9    0900  0910  0970  1023  1070
 R     1930
 R2    2750  2810  2940
 R[    0090  2020  2090  2140  2220  2230  2240  2260  2280  2320
       2340  2430  2440  2580
 T     1940
 T$    0100  0160  0166  0235  0999  1850  2610  2970
 T[    0090  2020  2030  2050
 V$    0100  0170  0330  0340  0350  1040  1041  1100  1140  2160
       2180  2190
 V0$   0090  0910  0920  0950
 X     1450  1460  1465  1470  1475  1500  1520  1820  1980  2010
       2020  2050  2070  2080  2120  2130  2210  2270  2300  2330
       2430  2440  2580  2940
 X$    0100  0240  0250  0360  0370
 Z     1021  1065
 Z3    2260  2280  2320  2340
```

SECTION 8

PROGRAM GC06 - CALIBRATION CURVE PLOTTING

GC06 is the program which draws a calibration curve and prints a table of residuals. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed. The plotting features of this program are written exclusively for a Tektronix 4000 Series Computer Display Terminal, or a Hewlett-Packard 2647 or 2648 terminal in Tektronix compatability mode. However, the program is designed so that it can print all of the calibration information except the plot itself on a non-Tektronix terminal.

This program uses a set of general purpose BASIC Tektronix plotting subroutines which were developed by the Advanced Instrumentation Section. Complete documentation for those subroutines is available from that office.

As GC06 begins, it asks the analyst what type of terminal is being used. It then asks the user for the number of the method. It checks whether any such method file exists. The program then opens the method file and counts the number of identifiers in that file.

Next, the program asks the user for the identifier whose calibration curve is to be plotted, and it searches the method file for that identifier. When it finds the appropriate identifier, it reads all of the calibration data for that identifier from the method file.

Then, on a Tektronix-type terminal, the program clears the screen by printing "<27><12>" and DELAYing one second to allow the screen to physically clear. Then it prints the headings for the calibration curve plot. The program uses subroutine BSCPLT.SR to establish the origin at a random location within five addressable points of the lower left corner of the screen. This causes each graph to be drawn in a slightly different location so that the screen will wear more evenly.

Next, the program uses subroutine BSCAXS.SR four times to draw the four sides of the box. The axes are then identified.

The subroutine BSCSCL.SR is then used to generate numbers which scale the horizontal and vertical axes.

Next, the subroutine BSCMKR.SR is used to mark the calibration standards on the chart. If the type of curve fitting is linear interpolation, BSCMKR.SR also connects the points with straight line segments. For any of the other types of curve fitting, GC06 uses subroutine BSCLIN.SR to draw the curve. The bell is then sounded five times to tell the user that the drawing is complete. A TINPUT statement then causes GC06 to wait while the user makes a hard copy of the calibration curve. The program continues when the user presses the RETURN key or when the sixty seconds allowed for the TINPUT are over.

Next, the program prints the table of residuals, and it again sounds the bell five times and waits while the user makes a hard copy.

Finally, if the user wants to produce another graph, the program branches back to begin again. Otherwise, the program disables the escape feature and chains back to GC00.

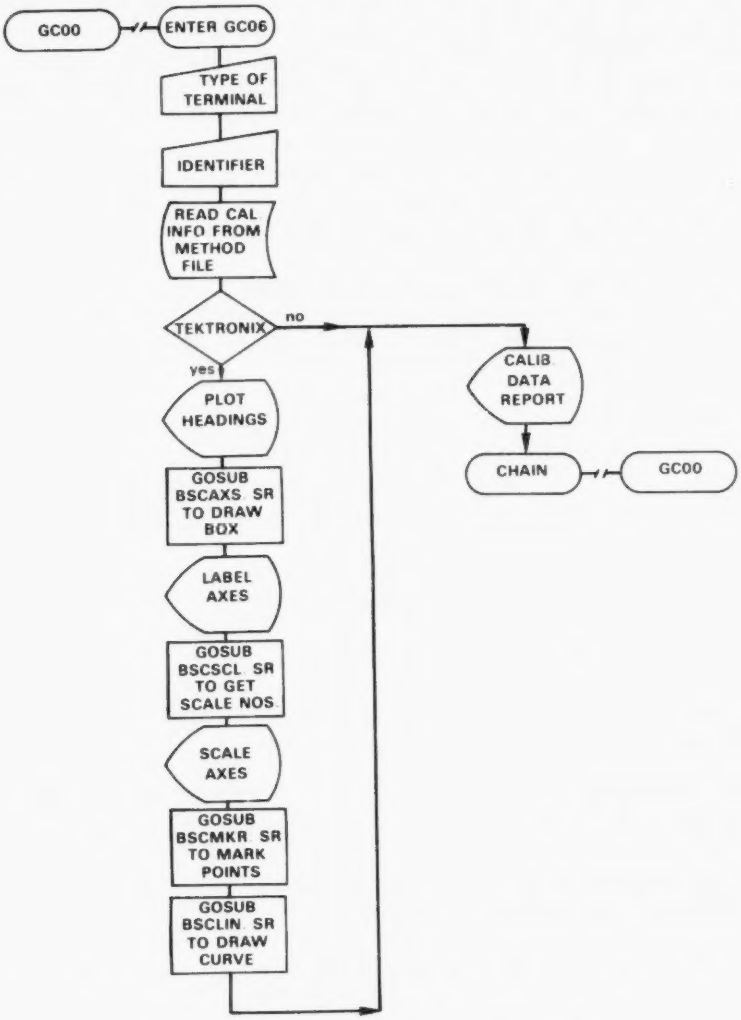

GC00
ENTER GC06
TYPE OF TERMINAL
IDENTIFIER
READ CAL INFO FROM METHOD FILE
TEKTRONIX
no
yes
PLOT HEADINGS
GOSUB BSCAXS.SR TO DRAW BOX
LABEL AXES
GOSUB BSCSCL.SR TO GET SCALE NOS.
SCALE AXES
GOSUB BSCMKR.SR TO MARK POINTS
GOSUB BSCLIN.SR TO DRAW CURVE
CALIB. DATA REPORT
CHAIN
GC00

Figure 7. Flowchart of Program GC06.

TABLE 5. SYMBOL DEFINITIONS FOR PROGRAM GC06

D4$	the date of calibration
G2()	the array of prepared concentrations and peak areas
I	the control variable for loops
I$	the superstring of injection IDs of standards used
I5	the number of identifiers in the method file
J3	the fitting error
K	the type of fit K=1 linear regression K=2 quadratic regression K=3 linear interpolation K=4 linear regression forced through the origin
L2	the calculated concentration of a standard
N1	the type of processing and calibration
P1	see BSCPLT.SR
P1$	see BSCPLT.SR
P2	see BSCPLT.SR
P2$	see BSCPLT.SR
P3	see BSCPLT.SR
P3$	see BSCPLT.SR
P4	see BSCPLT.SR
P4$	see BSCPLT.SR
P5	see BSCPLT.SR
P5$	see BSCMKR.SR

TABLE 5. (continued)

P6	see BSCPLT.SR
P7	see BSCPLT.SR
P8	see BSCPLT.SR
P9	see BSCPLT.SR
P()	see BSCLIN.SR
Q1	see BSCAXS.SR
Q2	see BSCAXS.SR
Q3	see BSCAXS.SR and BSCLIN.SR
Q4	see BSCAXS.SR
Q5	see BSCAXS.SR
Q5$	the format of a PRINT USING statement
Q6	see BSCAXS.SR
Q7	see BSCLIN.SR
Q8	see BSCLIN.SR
Q9	see BSCLIN.SR
Q()	see BSCLIN.SR
R1	the constant term of the regression equation
R2	the coefficient of the linear term of the regression equation
R3	the coefficient of the quadratic term of the regression equation
S$	the axis identification string
S1	see BSCSCL.SR
S2	see BSCSCL.SR
S3	see BSCSCL.SR
S4	see BSCSCL.SR

TABLE 5. (continued)

S5	see BSCSCL.SR
S6	see BSCSCL.SR
S7	see BSCSCL.SR
S()	see BSCSCL.SR
T$	the name of the method file
U$	the name of the analyst
U1	see BSCMKR.SR
U2	see BSCMKR.SR
U3	see BSCMKR.SR
V$	an identifier in a method file
V7$	the identifier to be plotted
X$	the user's answer to a Y or N question
X7	the x-coordinate of a point of the curve
X8	the x-coordinate of the left side of the box
X9	the x-coordinate of the right side of the box
Y8	the y-coordinate of the bottom of the box
Y9	the y-coordinate of the top of the box
Z5	the position of a slash in a string

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  1
                    PROGRAM LISTING FOR GC06

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                       +
0030 REM   +   PROGRAM GC06, CALIBRATION CURVE PLOTTING                   +
0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 6, 1979                      +
0045 REM   +   MOST RECENT REVISION:  MAY 8, 1979                         +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 DIM D4$[8],G2[30],I$[160],P[100],Q5$[75],Q[100],S$[40],T$[6]
0080 DIM U$[20],V$[8],V7$[8],X$[3]
0090 PAGE =132
0100 ON ESC THEN GOTO 3130
0110 ESC
0120 PRINT
0121 PRINT "HERE ARE THE TYPES OF TERMINALS:"
0122 PRINT
0123 PRINT "     1.  TEKTRONIX 4000 SERIES"
0124 PRINT "     2.  HEWLETT-PACKARD 2647 OR 2648"
0125 PRINT "     3.  ALL OTHER TERMINALS"
0126 PRINT
0130 ON ERR THEN GOTO 0150
0140 INPUT "WHICH TYPE OF TERMINAL ARE YOU USING?  (1, 2, OR 3)  ",X
0150 ON ERR THEN STOP
0151 IF X=ABS(INT(X)) THEN IF X>0 THEN IF X<4 THEN GOTO 0160
0152 PRINT
0153 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
0154 GOTO 0120
0160 IF X<>3 THEN GOTO 0210
0170 PRINT
0180 PRINT "THE PLOTTING FEATURES OF THIS OPTION WILL BE SKIPPED."
0200 GOTO 0260
0210 GOSUB 9905
0220 REM   ----------------------------------------------------------------
0230 REM             OPEN METHOD FILE
0260 READ FILE[4,1],T$
0270 CLOSE FILE[4]
0280 OPEN FILE[4,0],T$,200
0540 REM   ----------------------------------------------------------------
0550 REM             COUNT IDENTIFIERS IN METHOD FILE
0560 LET I5=1
0570 READ FILE[4,3*I5-1],V$
0580 IF EOF(4) THEN GOTO 0610
0590 LET I5=I5+1

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  2
                    PROGRAM LISTING FOR GC06

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0600 GOTO 0570
0610 LET I5=I5-1
0620 REM   ----------------------------------------------------------------
0630 REM             INPUT IDENTIFIER TO BE PLOTTED
0640 PRINT
0645 PRINT "WHAT IDENTIFIER FROM METHOD ";T$[3,6];
0650 ON ERR THEN GOTO 0720
0660 INPUT " DO YOU WANT CALIBRATION DATA FOR?  ",V7$
0670 ON ERR THEN STOP
0680 LET Z5=POS(V7$,"/",1)
0690 IF Z5=0 THEN GOTO 0780
0700 LET V7$[Z5,Z5]=","
0710 GOTO 0680
0720 ON ERR THEN STOP
0730 PRINT
0740 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
0750 GOTO 0640
0760 REM   ----------------------------------------------------------------
0770 REM             CHECK IF IDENTIFIER IS IN METHOD FILE
0780 FOR I=1 TO I5
0800   READ FILE[4,3*I-1],V$
0810   IF V$=V7$ THEN GOTO 0880
0820 NEXT I
0830 PRINT
0840 PRINT "<7><7>THERE IS NO IDENTIFIER '";V7$;"' IN METHOD ";T$[3,6]
*     ;"."
0850 GOTO 0640
0860 REM   ----------------------------------------------------------------
0870 REM             READ DATA FROM METHOD FILE
0880 READ FILE[4,3*I],D4$,I$,K,R1,R2,R3,J3
0890 IF D4$<>"99/99/99" THEN GOTO 0930
0900 PRINT
0910 PRINT "<7><7>IDENTIFIER ";V7$;" HAS NEVER BEEN CALIBRATED."
0920 GOTO 0640
0930 MAT READ FILE[4,3*I+1],G2
0940 READ FILE[4,1],T$,U$,N1
0950 REM   ----------------------------------------------------------------
0960 REM             CLEAR SCREEN, PRINT HEADINGS
0970 IF X=3 THEN GOTO 2530
0971 IF X<>2 THEN GOTO 0980
0972 PRINT "<27>*DF"
0973 PRINT "<27>&S1P0Q"

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  3
                       PROGRAM LISTING FOR GC06

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0980 PRINT "<27><12>";
0990 DELAY =1
1000 PRINT  TAB(22);"GAS CHROMATOGRAPHY AUTOMATION SYSTEM"
1010 PRINT  TAB(20);" C-A-L-I-B-R-A-T-I-O-N    C-U-R-V-E"
1020 PRINT "ANALYST:  ";U$; TAB(60);"METHOD:  ";T$[3,6]
1030 PRINT "IDENTIFIER:  ";V7$; TAB(43);"DATE OF CALIBRATION:  ";D4$
1040 PRINT "TYPE OF FIT:  ";
1050 ON K THEN GOTO 1060, 1080, 1100, 1120
1060 PRINT "LINEAR REGRESSION";
1070 GOTO 1130
1080 PRINT "QUADRATIC REGRESSION";
1090 GOTO 1130
1100 PRINT "LINEAR INTERPOLATION";
1110 GOTO 1130
1120 PRINT "LINEAR REGRESSION THROUGH ORIGIN";
1130 PRINT  TAB(51);
1140 PRINT USING "FITTING ERROR: ###.##%",J3
1150 REM   ------------------------------------------------------------
1160 REM           DRAW BOX
1170 RANDOMIZE
1180 LET P1=RND(1)*5
1190 LET P2=RND(2)*5
1200 LET P3=0
1210 GOSUB 9968
1220 LET Q1=147
1230 LET Q2=70
1240 LET Q3=11
1250 LET Q4=78
1260 LET Q5=2
1270 GOSUB 9924
1280 LET Q4=54
1290 LET Q5=1
1300 GOSUB 9924
1310 LET Q2=664
1320 LET Q4=78
1330 LET Q5=-2
1340 GOSUB 9924
1350 LET Q1=1005
1360 LET Q2=70
1370 LET Q4=54
1380 LET Q5=-1
1390 GOSUB 9924

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  4
                       PROGRAM LISTING FOR GC06

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1400 REM   ------------------------------------------------------------
1410 REM            LABEL AXES
1420 LET P1=0
1430 LET P2=500
1440 LET P3=3
1450 GOSUB 9968
1460 LET S$="PEAK AREA"
1470 FOR I=1 TO LEN(S$)
1480   PRINT S$[I,I];"<13>";
1490 NEXT I
1500 LET P1=0
1510 LET P2=0
1520 LET P3=3
1530 GOSUB 9968
1540 LET S$="CONCENTRATION IN MICROGRAMS PER LITER"
1550 IF N1>2 THEN LET S$="             MASS IN NANOGRAMS"
1560 PRINT "<29>";P4$;"<31>"; TAB(28);S$
1570 REM   ------------------------------------------------------------
1580 REM            SCALE VERTICAL AXIS
1590 LET S1=0
1600 LET S2=0
1610 FOR I=1 TO LEN(I$)/8
1620   IF G2[2*I]>S2 THEN LET S2=G2[2*I]
1630 NEXT I
1640 GOSUB 9805
1650 LET Y8=S[1]
1660 LET Y9=S[12]
1670 LET P1=0
1680 LET P3=3
1690 FOR I=1 TO 12
1700   LET P2=58+(I-1)*54
1710   GOSUB 9968
1720   PRINT "<29>";P4$;"<31>";
1730   PRINT USING "##########",S[I]
1740 NEXT I
1750 REM   ------------------------------------------------------------
1760 REM            SCALE HORIZONTAL AXIS
1770 LET S1=0
1780 LET S2=0
1790 FOR I=1 TO LEN(I$)/8
1800   IF G2[2*I-1]>S2 THEN LET S2=G2[2*I-1]
1810 NEXT I

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC06

```
12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
1820 GOSUB 9805
1830 LET X8=S[1]
1840 LET X9=S[12]
1850 IF S[12]>=10 THEN GOTO 1880
1860 LET Q5$=" #.##"
1870 GOTO 1920
1880 IF S[12]>=100 THEN GOTO 1910
1890 LET Q5$=" ##.#"
1900 GOTO 1920
1910 LET Q5$="#####"
1920 LET P2=30
1930 FOR I=1 TO 12
1940   LET P1=105+(I-1)*78
1950   GOSUB 9968
1960   PRINT "<29>";P4$;"<31>";
1970   PRINT USING Q5$,S[I]
1980 NEXT I
1990 REM    -------------------------------------------------------------
2000 REM             DRAW MARKERS
2010 LET P4=P4+147
2020 LET P5=P5+70
2030 LET P5$="*"
2040 FOR I=1 TO LEN(I$)/8
2050   LET P[I]=858*(G2[2*I-1]-X8)/(X9-X8)
2060   LET Q[I]=594*(G2[2*I]-Y8)/(Y9-Y8)
2070 NEXT I
2080 LET Q3=LEN(I$)/8
2090 LET Q7=-1
2100 IF K<>3 THEN GOTO 2160
2110 LET Q7=1
2120 LET P1=0
2130 LET P2=0
2140 LET P3=3
2150 GOSUB 9968
2160 GOSUB 9881
2170 REM    -------------------------------------------------------------
2180 REM             DRAW CURVE
2190 IF K=3 THEN GOTO 2390
2200 LET Q3=1
2210 FOR I=Y8 TO .99*Y9 STEP (Y9-Y8)/100
2220   LET Q[Q3]=594*(I-Y8)/(Y9-Y8)
2230   LET X7=R1+R2*I

12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC06

```
12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
2240   IF K=2 THEN LET X7=X7+R3*I^2
2250   LET P[Q3]=858*(X7-X8)/(X9-X8)
2260   IF P[Q3]<0 THEN GOTO 2290
2270   IF P[Q3]>858 THEN GOTO 2290
2280   LET Q3=Q3+1
2290 NEXT I
2300 LET Q3=Q3-1
2310 LET P1=P[1]
2320 LET P2=Q[1]
2330 LET P3=3
2340 GOSUB 9968
2350 LET G7=0
2360 GOSUB 9881
2370 REM    -------------------------------------------------------------
2380 REM          SOUND THE BELL; ALLOW TIME FOR HARD COPY
2390 FOR I=1 TO 5
2400   PRINT "<7>"
2410   DELAY =.3
2420 NEXT I
2430 TIME =60
2440 ON ERR THEN GOTO 2460
2450 TINPUT "",X$
2460 ON ERR THEN STOP
2470 PRINT "<27><12>";
2480 DELAY =1
2482 IF X<>2 THEN GOTO 2490
2483 PRINT "<27>E"
2484 PRINT "<27>H<27>J"
2485 PRINT "<27>*DE"
2490 PRINT  TAB(15);"C-A-L-I-B-R-A-T-I-O-N   D-A-T-A   R-E-P-O-R-T"
2500 GOTO 2690
2510 REM    -------------------------------------------------------------
2520 REM             PRINT TABLE OF RESIDUALS
2530 PRINT
2540 PRINT
2550 PRINT  TAB(15);"C-A-L-I-B-R-A-T-I-O-N   D-A-T-A   R-E-P-O-R-T"
2560 PRINT "ANALYST:  ";U$; TAB(60);"METHOD:  ";T$[3,6]
2570 PRINT "IDENTIFIER:  ";V7$; TAB(43);"DATE OF CALIBRATION:  ";D4$
2580 PRINT "TYPE OF FIT:  ";
2590 ON K THEN GOTO 2600, 2620, 2640, 2660
2600 PRINT "LINEAR REGRESSION";
2610 GOTO 2670

12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
2620 PRINT "QUADRATIC REGRESSION";
2630 GOTO 2670
2640 PRINT "LINEAR INTERPOLATION";
2650 GOTJ 2670
2660 PRINT "LINEAR REGRESSION THROUGH ORIGIN";
2670 PRINT  TAB(51);
2680 PRINT USING "FITTING ERROR: ###.##%",J3
2690 PRINT
2700 PRINT "INJECTION ID  PEAK AREA   PREPARED   CALCULATED  DIFFERENC
*    E"
2710 PRINT "------------  ---------  ----------  ----------  ---------
*    -"
2720 LET Q5$="  ########   ########### -----#.### -----#.###   +++#.#
*    ##"
2730 FOR I=1 TO LEN(I$)/8
2740   ON K THEN GOTO 2750, 2770, 2790, 2750
2750   LET L2=R1+G2[I*2]*R2
2760   GOTO 2800
2770   LET L2=R1+G2[I*2]*R2+R3*G2[I*2]^2
2780   GOTO 2800
2790   LET L2=G2[I*2-1]
2800   PRINT USING Q5$,I$[8*I-7,8*I],G2[I*2],G2[I*2-1],L2,G2[I*2-1]-L2
2810 NEXT I
2820 IF K=3 THEN GOTO 3060
2830 PRINT
2840 PRINT "EQUATION:  CONCENTRATION = ";
2850 ON K THEN GOTO 2860, 2880, 3060, 2900
2860 PRINT USING "+#.##^^^^(A) +#.##^^^^",R2,R1
2870 GOTO 3060
2880 PRINT USING "+#.##^^^^(A^2) +#.##^^^^(A) +#.##^^^^",R3,R2,R1
2890 GOTO 3060
2900 PRINT USING "+#.##^^^^(A)",R2
3040 REM   ------------------------------------------------------------
3050 REM          RETURN TO MASTER CONTROL
3060 PRINT
3065 PRINT
3070 PRINT "DO YOU WANT CALIBRATION INFORMATION FOR ANOTHER IDENTIFIER
*    "
3080 PRINT "      IN METHOD ";T$[3,6];
3090 ON ERR THEN GOTO 3110
3100 INPUT "?  (Y OR N)  ",X$
3110 ON ERR THEN STOP

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
3120 IF X$[1,1]="Y" THEN GO'O 0640
3130 NOESC
3140 CHAIN "GC00"
9800 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9801 REM          SUBROUTINE TO PERFORM SCALING (BSCSCL.SR)
9805 DIM S[12]
9806 LET S7=0
9808 LET S3=S2-S1
9809 IF S3>=100 THEN GOTO 9815
9810 LET S1=S1*10
9811 LET S2=S2*10
9812 LET S7=S7+1
9813 GOTO 9808
9815 LET S4=0
9816 IF S3<100 THFN GOTO 9820
9817 LET S3=S3/10
9818 LET S4=S4+1
9819 GOTO 9816
9820 IF S1=0 THEN IF S3-10*INT(S3/10)<=INT(S3/10) THEN LET S3=10*INT(S
*    3/10)
9821 LET S3=INT(S3+.5)
9823 IF S3-10*INT(S3/10)=0 THEN GOTO 9828
9824 IF S3-10*INT(S3/10)=5 THEN GOTO 9828
9825 LET S3=S3+1
9826 GOTO 9823
9828 LET S5=S3*10^(S4-1)
9830 LET S1=INT(S1/10^(S4-1))*10^(S4-1)
9831 IF S1/S5=INT(S1/S5) THEN GOTO 9835
9832 LET S1=S1-10^(S4-1)
9833 GOTO 9831
9835 FOR S6=1 TO 12
9836   LET S[S6]=(S1+(S6-1)*S5)/10^(S7)
9837 NEXT S6
9838 RETURN
9875 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9876 REM          SUBROUTINE TO DRAW LINES AND CURVES (BSCLIN.SR)
9881 LET Q8=0
9882 LET P3=3
9885 IF Q7>=0 THEN LET P3=2
9886 FOR Q9=1 TO Q3
9887   LET P1=P[Q9]
9888   LET P2=Q[Q9]

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
9889   GOSUB 9968
9890   LET Q8=Q8+1
9891   IF Q8<>ABS(Q7) THEN GOTO 9896
9892   LET U1=P[Q9]
9893   LET U2=Q[Q9]
9894   GOSUR 9908
9895   LET Q8=0
9896 NEXT Q9
9897 RETURN
9900 REM    +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9901 REM           SUBROUTINE TO PLACE MARKERS (BSCMKR.SR)
9905 DIM P5$[10]
9906 GOSUB 9958
9907 RETURN
9908 LET P1=U1-5
9909 LET P2=U2-8
9910 LET U3=P3
9911 LET P3=3
9912 GOSUR 9968
9913 PRINT "<29>";P4$;
9914 PRINT "<31>";P5$[1,LEN(P5$)]
9915 LET P1=U1
9916 LET P2=U2
9917 GOSUB 9968
9918 LET P3=U3
9919 RETURN
9920 REM    +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9921 REM           SUBROUTINE TO DRAW AXES (BSCAXS.SR)
9924 LET P1=Q1
9925 LET P2=Q2
9926 LET P3=3
9927 GOSUB 9968
9928 LET P3=2
9929 IF ABS(Q5)=1 THEN GOTO 9939
9930 FOR Q6=1 TO Q3+1
9931   GOSUB 9968
9932   LET P2=P2+10*Q5/ABS(Q5)
9933   GOSUB 9968
9934   LET P2=P2-10*Q5/ABS(Q5)
9935   GOSUB 9968
9936   LET P1=P1+Q4
9937 NEXT Q6

12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
9938 RETURN
9939 FOR Q6=1 TO Q3+1
9940   GOSUB 9968
9941   LET P1=P1+10*Q5/ABS(Q5)
9942   GOSUB 9968
9943   LET P1=P1-10*Q5/ABS(Q5)
9944   GOSUB 9968
9945.  LET P2=P2+Q4
9946 NEXT Q6
9947 RETURN
9950 REM    +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9951 REM           SUBROUTINE TO PLOT INDIVIDUAL POINTS (BSCPLT.SR)
9958 DIM P1$[32],P2$[32],P3$[32],P4$[4]
9959 LET P4=0
9960 LET P5=0
9961 LET P6=0
9962 LET P1$=" !<34>#$%&'()*+,-./0123456789:;<=>?"
9963 LET P2$="@ABCDEFGHIJKLMNOPQRSTUVWXYZ[\]^_"
9964 LET P3$="`ABCDEFGHIJKLM"
9965 LET P3$=P3$,"NOPQRSTUVWXY"
9966 LET P3$=P3$,"Z[\]^"
9967 RETURN
9968 IF P3<>0 THEN GOTO 9972
9969 LET P4=P1
9970 LET P5=P2
9971 RETURN
9972 PRINT "<29>";
9973 IF LEN(P4$)<>0 THEN PRINT P4$[4,4];
9974 LET P7=INT(P1+P4)
9975 LET P8=INT(P2+P5)
9976 IF P7>1023 THEN LET P7=1023
9977 IF P7<0 THEN LET P7=0
9978 IF P8>780 THEN LET P8=780
9979 IF P8<0 THEN LET P8=0
9980 IF P3=2 THEN LET P6=1
9981 IF P3=3 THEN LET P6=0
9982 LET P9=INT(P8/32)
9983 LET P8=P8-(P9*32)+1
9984 LET P9=P9+1
9985 LET P4$=P1$[P9,P9],P3$[P8,P8]
9986 LET P9=INT(P7/32)
9987 LET P7=P7-(P9*32)+1

12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE 11
                     PROGRAM LISTING FOR GC06

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
9988 LET P9=P9+1
9989 LET P4$=P4$,P1$[P9,P9],P2$[P7,P7]
9990 IF P6<>0 THEN GOTO 9992
9991 PRINT "<29>";
9992 PRINT P4$
9993 RETURN

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE 12
                         SYMBOL TABLE FOR GC06

SYMBOL    REFERENCES
------ ---------------------------------------------------------------
 0120  0154
 0150  0130
 0160  0151
 0210  0160
 0260  0200
 0570  0600
 0610  0580
 0640  0750  0850  0920  3120
 0680  0710
 0720  0650
 0780  0690
 0880  0810
 0930  0890
 0980  0971
 1060  1050
 1080  1050
 1100  1050
 1120  1050
 1130  1070  1090  1110
 1880  1850
 1910  1880
 1920  1870  1900
 2160  2100
 2290  2260  2270
 2390  2190
 2460  2440
 2490  2482
 2530  0970
 2600  2590
 2620  2590
 2640  2590
 2660  2590
 2670  2610  2630  2650
 2690  2500
 2750  2740
 2770  2740
 2790  2740
 2800  2760  2780
 2860  2850
 2880  2850
 2900  2850
 3060  2820  2850  2870  2890
 3110  3090
 3130  0100
 9805  1640  1820
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE 13
                          SYMBOL TABLE FOR GC06

SYMBOL   REFERENCES
------   ---------------------------------------------------------------
 9808    9813
 9815    9809
 9816    9819
 9820    9816
 9823    9826
 9828    9823  9824
 9831    9833
 9835    9831
 9881    2160  2360
 9896    9891
 9905    0210
 9908    9894
 9924    1270  1300  1340  1390
 9939    9929
 9958    9906
 9968    1210  1450  1530  1710  1950  2150  2340  9889  9912  9917
         9927  9931  9933  9935  9940  9942  9944
 9972    9968
 9992    9990
 D4$     0070  0880  0890  1030  2570
 FL#4    0260  0270  0280  0570  0800  0880  0930  0940
 G2      0930
 G2[     0070  1620  1800  2050  2060  2750  2770  2790  2800
 I       0780  0800  0820  0880  0930  1470  1480  1490  1610  1620
         1630  1690  1700  1730  1740  1790  1800  1810  1930  1940
         1970  1980  2040  2050  2060  2070  2210  2220  2230  2240
         2290  2390  2420  2730  2750  2770  2790  2800  2810
 I$      0070  0880  1610  1790  2040  2080  2730  2800
 I5      0560  0570  0590  0610  0780
 J3      0880  1140  2680
 K       0880  1050  2100  2190  2240  2590  2740  2820  2850
 L2      2750  2770  2790  2800
 N1      0940  1550
 P1      1180  1420  1500  1670  1940  2120  2310  9887  9908  9915
         9924  9936  9941  9943  9969  9974
 P1$     9958  9962  9985  9989
 P2      1190  1430  1510  1700  1920  2130  2320  9888  9909  9916
         9925  9932  9934  9945  9970  9975
 P2$     9958  9963  9989
 P3      1200  1440  1520  1680  2140  2330  9882  9885  9910  9911
         9918  9926  9928  9968  9980  9981
 P3$     9958  9964  9965  9966  9985
 P4      2010  9959  9969  9974
 P4$     1560  1720  1960  9913  9958  9973  9985  9989  9992
 P5      2020  9960  9970  9975
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE 14
                          SYMBOL TABLE FOR GC06

SYMBOL   REFERENCES
------   ---------------------------------------------------------------
 P5$     2030  9905  9914
 P6      9961  9980  9981  9990
 P7      9974  9976  9977  9986  9987  9989
 P8      9975  9978  9979  9982  9983  9985
 P9      9982  9983  9984  9985  9986  9987  9988  9989
 P[      0070  2050  2250  2260  2270  2310  9887  9892
 Q1      1220  1350  9924
 Q2      1230  1310  1360  9925
 Q3      1240  2080  2200  2220  2250  2260  2270  2280  2300  9886
         9930  9939
 Q4      1250  1280  1320  1370  9936  9945
 Q5      1260  1290  1330  1380  9929  9932  9934  9941  9943
 Q5$     0070  1860  1890  1910  1970  2720  2800
 Q6      9930  9937  9939  9946
 Q7      2090  2110  2350  9885  9891
 Q8      9881  9890  9891  9895
 Q9      9886  9887  9888  9892  9893  9896
 Q[      0070  2060  2220  2320  9888  9893
 R1      0880  2230  2750  2770  2860  2880
 R2      0880  2230  2750  2770  2860  2880  2900
 R3      0880  2240  2770  2880
 S$      0070  1460  1470  1480  1540  1550  1560
 S1      1590  1770  9808  9810  9820  9830  9831  9832  9836
 S2      1600  1620  1780  1800  9808  9811
 S3      9808  9809  9816  9817  9820  9821  9823  9824  9825  9828
 S4      9815  9818  9828  9830  9832
 S5      9828  9831  9836
 S6      9835  9836  9837
 S7      9806  9812  9836
 S[      1650  1660  1730  1830  1840  1850  1880  1970  9805  9836
 T$      0070  0260  0280  0645  0840  0940  1020  2560  3080
 U$      0080  0940  1020  2560
 U1      9892  9908  9915
 U2      9893  9909  9916
 U3      9910  9918
 V$      0080  0570  0800  0810
 V7$     0080  0660  0680  0700  0810  0840  0910  1030  2570
 X       0140  0151  0153  0160  0970  0971  2482
 X$      0080  2450  3100  3120
 X7      2230  2240  2250
 X8      1830  2050  2250
 X9      1840  2050  2250
 Y8      1650  2060  2210  2220
 Y9      1660  2060  2210  2220
 Z5      0680  0690  0700
```

SECTION 9

PROGRAM GC07 - EXTANT INJECTION LISTING

GC07 is the program which lists the injection ID numbers and report titles for the data files that are currently in existence. This program is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

As GC07 begins, it gives the user three choices: 1) print all extant ID numbers for one instrument, 2) print ID numbers for a specific date for one instrument, or 3) print the report title for any ID from any instrument. The program then branches to the appropriate routine.

The first two choices involve reading ID numbers from an ID list file. GC07 asks the user for the number of the instrument, and uses this number to generate the name of the appropriate ID list file. It then checks whether the ID list file exists. The ID list file must be opened carefully since the microcomputer may be running GC21 which also opens ID list files. Therefore, GC07 establishes an OR ERR THEN GOTO condition, opens the ID list file, copies the entire file into a superstring, and promptly closes the file to avoid making the microcomputer wait.

Then, if the user has selected the first type of report, GC07 prints all of the ID numbers, except dummy ID numbers. If the user has selected the second type of report, GC07 asks for a month and date, and prints only those ID numbers which match the specified month and date. If none of the ID numbers match, the user is informed of that fact.

The third type of report is different from the other two in that it gets the report title from an injection data file. The user is asked for the ID number of interest, and GC07 opens the appropriate data file. It finds the report title and prints it. The program then gives the user a chance to examine another file.

After any of these types of reports, the escape feature is disabled, and the program chains back to GC00.

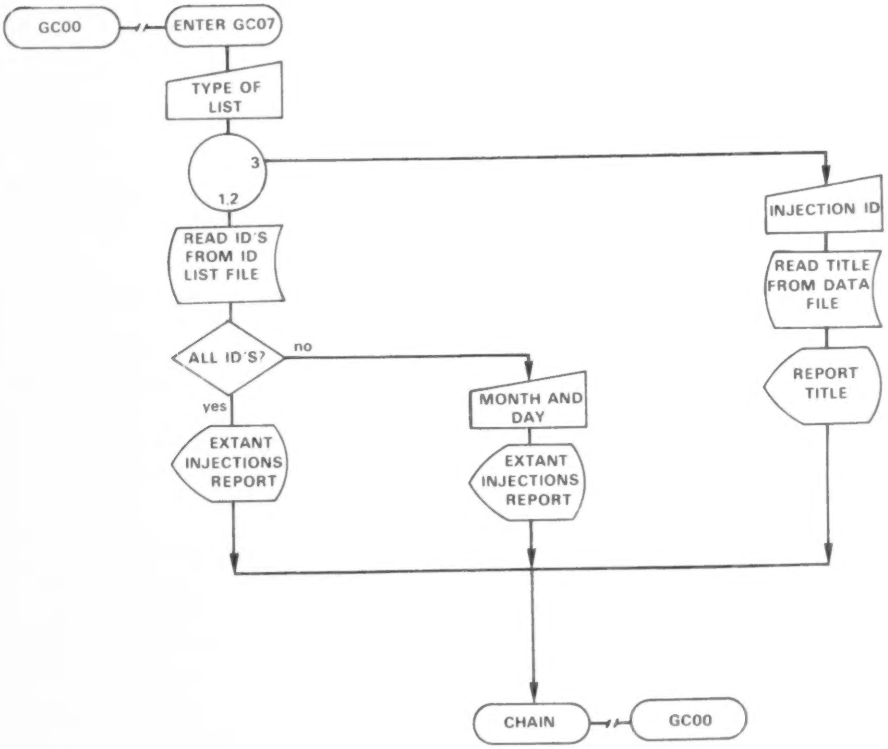

GC00
ENTER GC07
TYPE OF LIST
3
1,2
READ ID'S FROM ID LIST FILE
ALL ID'S?
no
yes
EXTANT INJECTIONS REPORT
MONTH AND DAY
EXTANT INJECTIONS REPORT
INJECTION ID
READ TITLE FROM DATA FILE
REPORT TITLE
CHAIN
GC00

Figure 8. Flowchart of Program GC07.

TABLE 6. SYMBOL DEFINITIONS FOR PROGRAM GC07

C$	the name of the ID list file
D2$	an injection ID Number
D3$	a data file name
E	a counter for the number of ID Numbers which match the specified date
F$	a report title
I	the control variable for loops
I$	the superstring of extant ID numbers
J	the data file useability flag
J$	the date of an injection, in the form MMDD
X	the user's answer to a multiple choice question
X$	a Y or N answer input by the user
X2	the instrument number input by the user
X3	the month and date numbers input by the user

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE 1
                       PROGRAM LISTING FOR GC07

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                     +
0030 REM   +   PROGRAM GC07, DATA FILE LISTING                          +
0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 23, 1979                 +
0045 REM   +   MOST RECENT REVISION:  MAY 1, 1979                       +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 1460
0090 DIM C$[8],D2$[8],D3$[10],F$[30],I$[1000],J$[4],X$[3]
0120 REM   ---------------------------------------------------------------
0130 REM           DEFINE SEARCH
0140 PRINT
0150 PRINT "HERE ARE THE TYPES OF LISTS:"
0160 PRINT
0170 PRINT "     1.  ALL EXTANT ID NUMBERS FROM ONE INSTRUMENT"
0180 PRINT "     2.  ID NUMBERS FOR A SPECIFIC DATE FROM ONE INSTRUMEN
*    T"
0190 PRINT "     3.  TITLE OF REPORT FOR ANY ID FROM ANY INSTRUMENT"
0200 PRINT
0205 ON ERR THEN GOTO 0215
0210 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, OR 3)  ",X
0215 ON ERR THEN STOP
0220 ON X THEN GOTO 0260, 0260, 0920
0230 PRINT
0240 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
0250 GOTO 0140
0255 REM   ---------------------------------------------------------------
0256 REM           COPY ID LIST FILE INTO SUPERSTRING
0260 PRINT
0265 ON ERR THEN GOTO 0271
0270 INPUT "WHAT INSTRUMENT NUMBER?  ",X2
0271 ON ERR THEN STOP
0272 IF X2=ABS(INT(X2)) THEN IF X2<=99 THEN GOTO 0280
0273 PRINT
0274 PRINT "<7><7>";X2;"IS NOT A VALID INSTRUMENT NUMBER."
0275 GOTO 0260
0280 LET C$="GC000000"
0290 LET C$[9-LEN(STR$(X2)),8]=STR$(X2)
0300 ON ERR THEN GOTO 0320
0310 RENAME C$,C$
0320 ON ERR THEN STOP

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE 2
                       PROGRAM LISTING FOR GC07

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
0330 IF SYS(7)<>-48 THEN GOTO 0360
0340 DELAY =1
0350 GOTO 0300
0360 IF SYS(7)=-9 THEN GOTO 0400
0370 PRINT
0380 PRINT "THERE HAVE NOT BEEN ANY INJECTIONS INTO INSTRUMENT ";C$[7,
*    8];"."
0390 GOTO 1460
0400 ON ERR THEN GOTO 0460
0410 OPEN FILE[2,0],C$,11
0420 ON ESC THEN GOTO 0500
0430 ON ERR THEN STOP
0440 GOTO 0530
0460 ON ERR THEN STOP
0470 DELAY =1
0480 GOTO 0400
0500 CLOSE FILE[2]
0510 GOTO 1460
0530 FOR I=1 TO 100
0540   READ FILE[2,I],I$[10*I-9,10*I]
0550 NEXT I
0560 CLOSE FILE[2]
0570 ON ESC THEN GOTO 1460
0580 IF X=2 THEN GOTO 0700
0590 REM   ---------------------------------------------------------------
0600 REM           PRINT ALL ID NUMBERS
0610 PRINT
0611 PRINT
0612 PRINT  TAB(14);"E-X-T-A-N-T   I-N-J-E-C-T-I-O-N-S   R-E-P-O-R-T"
0613 PRINT "INSTRUMENT NUMBER:  ";C$[7,8]; TAB(59);"ALL INJECTIONS"
0614 PRINT
0620 FOR I=1 TO 100
0630   IF I$[10*I-9,10*I]="GC99999999" THEN GOTO 0670
0640   PRINT I$[10*I-7,10*I];
0645   IF I/6<>INT(I/6) THEN PRINT "     ";
0650   IF I/6=INT(I/6) THEN PRINT
0660 NEXT I
0670 GOTO 1460
0680 REM   ---------------------------------------------------------------
0690 REM           PRINT ID NUMBERS MATCHING A DATE
0700 PRINT
0705 ON ERR THEN GOTO 0711

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                         PAGE  3
                         PROGRAM LISTING FOR GC07

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0710 INPUT "WHAT MONTH?  (1, 2, 3, . . . . , OR 12)  ",X3
0711 ON ERR THEN STOP
0712 IF X3=ABS(INT(X3)) THEN IF X3<=12 THEN GOTO 0720
0713 PRINT
0714 PRINT "<7><7>";X3;"IS NOT A VALID MONTH."
0715 GOTO 0700
0720 LET J$="0000"
0730 LET J$[3-LEN(STR$(X3)),2]=STR$(X3)
0740 PRINT
0745 ON ERR THEN GOTO 0751
0750 INPUT "WHAT DATE?  (1, 2, 3, . . . . , OR 31)  ",X3
0751 ON ERR THEN STOP
0752 IF X3=ABS(INT(X3)) THEN IF X3<=31 THEN GOTO 0760
0753 PRINT
0754 PRINT "<7><7>";X3;"IS NOT A VALID DATE."
0755 GOTO 0740
0760 LET J$[5-LEN(STR$(X3)),4]=STR$(X3)
0770 PRINT
0771 PRINT
0772 PRINT  TAB(14);"E-X-T-A-N-T   I-N-J-E-C-T-I-O-N-S   R-E-P-O-R-T"
0773 PRINT "INSTRUMENT NUMBER:  ";C$[7,8];"                    MONTH:  ";J
*     $[1,2];"                     DAY:  ";J$[3,4]
0775 PRINT
0780 LET E=0
0790 FOR I=1 TO 100
0800   IF I$[10*I-5,10*I-2]<>J$ THEN GOTO 0840
0810   PRINT I$[10*I-7,10*I];
0820   LET E=E+1
0825   IF E/6<>INT(E/6) THEN PRINT "     ";
0830   IF E/6=INT(E/6) THEN PRINT
0840 NEXT I
0850 IF E<>0 THEN GOTO 1460
0870 PRINT "NONE"
0890 GOTO 1460
0900 REM  ----------------------------------------------------------
0910 REM          PRINT VARIAN REPORT TITLE FOR A SPECIFIC ID
0920 PRINT
0925 ON ERR THEN GOTO 0935
0930 INPUT "WHAT ID?  ",D2$
0935 ON ERR THEN STOP
0940 IF LEN(D2$)<>8 THEN GOTO 1030
0945 IF D2$="00000000" THEN GOTO 1030

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                         PAGE  4
                         PROGRAM LISTING FOR GC07

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0950 LET D3$="GC",D2$
0960 ON ERR THEN GOTO 0980
0970 RENAME D3$,D3$
0980 ON ERR THEN STOP
0990 IF SYS(7)<>-48 THEN GOTO 1020
1000 DELAY =1
1010 GOTO 0960
1020 IF SYS(7)=-9 THEN GOTO 1090
1030 PRINT
1040 PRINT "THERE IS NO EXISTING DATA FOR INJECTION ";D2$;"."
1050 GOTO 1410
1090 ON ERR THEN GOTO 1150
1100 OPEN FILE[3,0],D3$,31
1110 ON ESC THEN GOTO 1190
1120 ON ERR THEN STOP
1130 GOTO 1220
1150 ON ERR THEN STOP
1160 DELAY =1
1170 GOTO 1090
1190 CLOSE FILE[3]
1200 GOTO 1460
1220 READ FILE[3,1],J
1230 IF J=1 THEN GOTO 1300
1240 PRINT
1250 IF J=2 THEN PRINT D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT
*      HAVE A TOTAL AREA."
1260 IF J=3 THEN PRINT D2$;" CANNOT BE USED BECAUSE THE REPORT WAS IN
*     THE WRONG FORMAT."
1270 CLOSE FILE[3]
1280 ON ESC THEN GOTO 1460
1290 GOTO 1410
1300 LET I=2
1310 READ FILE[3,I],F$
1320 IF F$[1,7]<>"MESSAGE" THEN GOTO 1350
1330 LET I=I+1
1340 GOTO 1310
1350 LET I=I+1
1360 READ FILE[3,I],F$
1370 CLOSE FILE[3]
1380 ON ESC THEN GOTO 1460
1390 PRINT
1400 PRINT "FOR ID ";D2$;", THE REPORT TITLE IS '";F$;".'"

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  5
                      PROGRAM LISTING FOR GC07

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 1410 PRINT
 1415 ON ERR THEN GOTO 1425
 1420 INPUT "DO YOU WANT TO PRINT THE TITLE FOR ANOTHER ID?  (Y OR N)
*      ",X$
 1425 ON ERR THEN STOP
 1430 IF X$[1,1]="Y" THEN GOTO 0920
 1440 REM  ------------------------------------------------------------
 1450 REM           CHAIN BACK TO GC00
 1460 PRINT
 1461 PRINT
 1462 NOESC
 1470 CHAIN "GC00"




 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  6
                          SYMBOL TABLE FOR GC07

SYMBOL   REFERENCES
------   ----------------------------------------------------------------
0140     0250
0215     0205
0260     0220  0275
0271     0265
0280     0272
0300     0350
0320     0300
0360     0330
0400     0360  0480
0460     0400
0500     0420
0530     0440
0670     0630
0700     0580  0715
0711     0705
0720     0712
0740     0755
0751     0745
0760     0752
0840     0800
0920     0220  1430
0935     0925
0960     1010
0980     0960
1020     0990
1030     0940  0945
1090     1020  1170
1150     1090
1190     1110
1220     1130
1300     1230
1310     1340
1350     1320
1410     1050  1290
1425     1415
1460     0080  0390  0510  0570  0670  0850  0890  1200  1280  1380
C$       0090  0280  0290  0310  0380  0410  0613  0773
D2$      0090  0930  0940  0945  0950  1040  1250  1260  1400
D3$      0090  0950  0970  1100
E        0780  0820  0825  0830  0850
F$       0090  1310  1320  1360  1400
FL#2     0410  0500  0540  0560
FL#3     1100  1190  1220  1270  1310  1360  1370
I        0530  0540  0550  0620  0630  0640  0645  0650  0660  0790
         0800  0810  0840  1300  1310  1330  1350  1360
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  7
                         SYMBOL TABLE FOR GC07

SYMBOL    REFERENCES
------  ---------------------------------------------------------------
 I$     0090  0540  0630  0640  0800  0810
 J      1220  1230  1250  1260
 J$     0090  0720  0730  0760  0773  0800
 X      0210  0220  0240  0580
 X$     0090  1420  1430
 X2     0270  0272  0274  0290
 X3     0710  0712  0714  0730  0750  0752  0754  0760
```

SECTION 10

PROGRAM GC08 - INTERNAL STANDARDS CONCENTRATION CALCULATION

The internal standards calibration method is a planned future enhancement of the GCAS, but it has not been implemented in Version I.

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  1
                   PROGRAM LISTING FOR GC08

1234567891123456789212345678931234567894123456789512345678961234567897
        0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC08, INTERNAL CALIBRATION PROCESSING           +
0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 10, 1979                +
0045 REM   +   MOST RECENT REVISION:  MARCH 21, 1979                   +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 9998
0090 PRINT
0110 PRINT "<7><7>INTERNAL STANDARDS PROCESSING IS NOT OPERATIONAL AT
*     THIS TIME."
9998 NOESC
9999 CHAIN "GC00"





1234567891123456789212345678931234567894123456789512345678961234567897
        0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  2
                   SYMBOL TABLE FOR GC08

SYMBOL    REFERENCES
------  -------------------------------------------------------------
 9998   0080
```

SECTION 11

PROGRAM GC09 - PURGE AND TRAP CONCENTRATION CALCULATION

GC09 is the program which calculates concentrations of compounds in samples prepared by the purge and trap method. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

As the execution of GC09 begins, the method file is already open. The program asks the user for the injection ID of the injection which is to be processed, and it opens the corresponding data file. The program checks the data file useability flag, and informs the user if the data file is unusable. It then displays any error messages which were in the original report.

Next, the program reads the data for a single peak from the data file. If the peak is an unexplained peak, a dummy concentration of -9999 is written into the data file, and the program goes on to the next peak.

For named peaks, the program searches the method file for a matching identifier. If there is no matching identifier, the user is informed that the concentration cannot be calculated, and a dummy concentration of -9999 is written into the data file.

If a matching identifier is found, the program checks whether the identifier has been calibrated. If it has not, the user is informed that the concentration cannot be calculated, and a dummy concentration of -9999 is written into the data file.

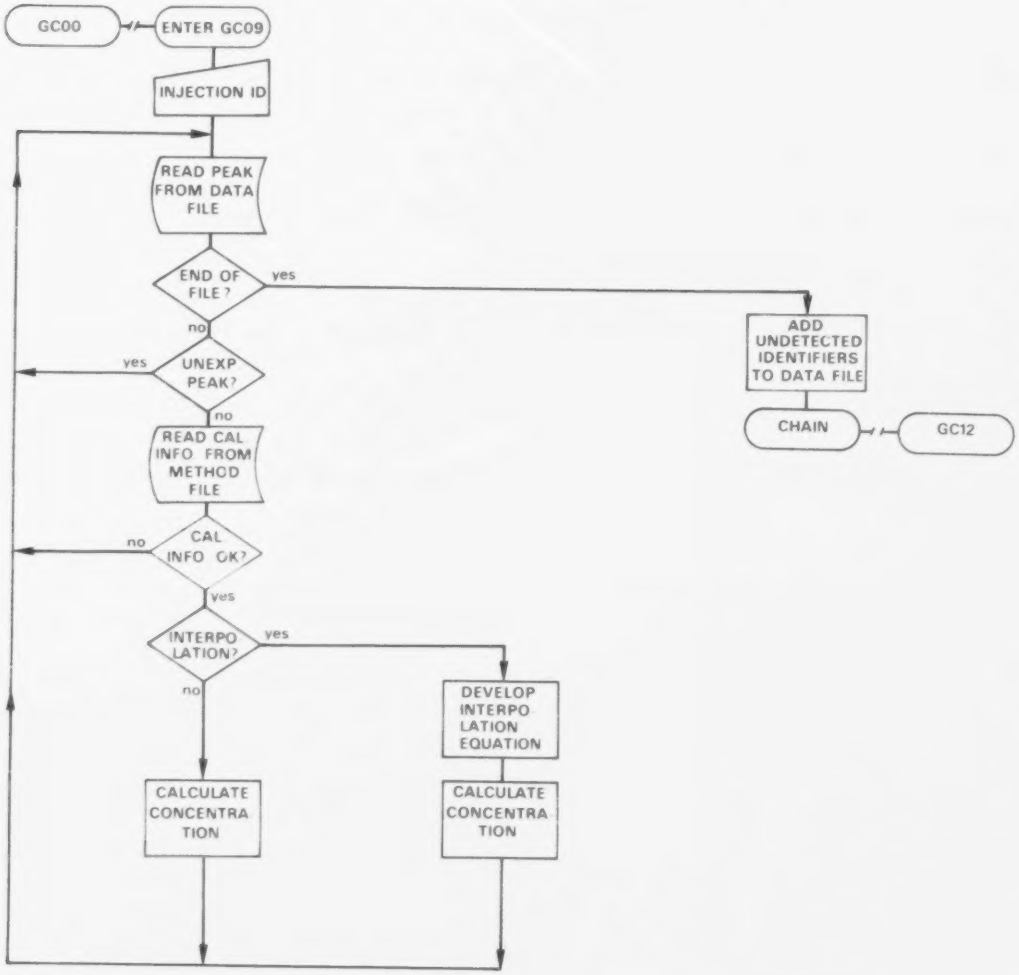
If the matching identifier has been calibrated, the program checks the type of calibration and branches to the appropriate section of code. If the type of calibration is linear regression or quadratic regression, the program uses the regression equations developed during calibration to calculate the concentration, which is written into the data file.

If the type of calibration is linear interpolation, the program finds the two calibration standards whose peak areas bracket the peak area of the unknown. If the peak area of the unknown is lower than that of the lowest calibration standard, the program uses the origin and the lowest calibration standard as the basis for the interpolation. If the peak area of the unknown is higher than that of the highest calibration standard, the program extrapolates through the two highest calibration standards. In any case, the concentration of the unknown is calculated by the formula

$$\text{Conc.} = \left(\frac{\text{Conc}_2 - \text{Conc}_1}{\text{Area}_2 - \text{Area}_1}\right)\left(\text{Area} - \text{Area}_1\right) + \left(\text{Conc}_1\right)$$

and written into the data file.

When all of the peaks in the data file have been processed, this program chains to the retention time calculation program, GC12, leaving the method file and the injection data file open.



GC00
ENTER GC09
INJECTION ID
READ PEAK FROM DATA FILE
END OF FILE?
yes
no
UNEXP PEAK?
yes
no
READ CAL INFO FROM METHOD FILE
CAL INFO OK?
no
yes
INTERPO LATION?
yes
no
DEVELOP INTERPO LATION EQUATION
CALCULATE CONCENTRA TION
CALCULATE CONCENTRA TION
ADD UNDETECTED IDENTIFIERS TO DATA FILE
CHAIN
GC12

Figure 9. Flowchart of Program GC09.

TABLE 7. SYMBOL DEFINITIONS FOR PROGRAM GC09

B	the absolute retention time of a peak
C	the area of a peak
D2$	an injection ID
D3$	the name of a data file
D4$	the date of calibration
F	the number of identifiers in the method file
F()	the array of flags used to record which identifiers are found in the data file
G$	the identifier from the data file
G2()	the array of concentrations and areas of standards
H$	the peak type
I	a counter used in interpolation to locate the standards between which the unknown lies
I$	the superstring of ID's of standards
I5	the number of standards used to calibrate an identifier
I7	a counter used to locate an identifier in a method file
J	the data file useability flag J=1 the data is useable J=2 the report did not have a TOTAL AREA J=3 the report was in the wrong format
J3	the fitting error of the regression
K	the type of fit K=1 linear regression K=2 quadratic regression K=3 linear interpolation K=4 linear regression forced through the origin

TABLE 7. (Continued)

L	the calculated relative retention time or capacity ratio
M1	the concentration of the standard below the unknown
M2	the area of the standard below the unknown
M3	the concentration of the standard above the unknown
M4	the area of the standard above the unknown
P9	a counter for the position in the data file of the peak being processed
R1	the constant term in the regression equation
R2	the linear term in the regression equation
R3	the quadratic term in the regression equation
T$	the name of the method file
V$	an identifier from the method file
VO$	a MESSAGE read from the data file

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                      PROGRAM LISTING FOR GC09

12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                      +
0030 REM   +   PROGRAM GC09, PURGE AND TRAP PROCESSING                   +
0040 REM   +   BY:  J. KOPKE (SWORCC), FEBRUARY 13, 1979                 +
0045 REM   +   MOST RECENT REVISION:  APRIL 2, 1979                      +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 0110
0090 DIM D2$[8],D3$[10],D4$[8],G$[8],G2[30],H$[2],I$[160],T$[6],V$[8],
*    V0$[20]
0095 DIM F[60]
0096 MAT F=ZER
0100 GOTO 0160
0110 ON ERR THEN GOTO 0112
0111 CLOSE FILE[3]
0112 ON ERR THEN STOP
0120 NOESC
0130 CHAIN "GC00"
0140 REM   ---------------------------------------------------------------
0150 REM          COUNT IDENTIFIERS IN METHOD FILE
0160 LET F=0
0170 READ FILE[4,1],T$
0175 CLOSE FILE[4]
0176 OPEN FILE[4,0],T$,200
0180 READ FILE[4,3*(F+1)-1],V$
0190 IF EOF(4) THEN GOTO 0240
0200 LET F=F+1
0210 GOTO 0180
0220 REM   ---------------------------------------------------------------
0230 REM          OPEN DATA FILE
0240 PRINT
0245 ON ERR THEN GOTO 0255
0248 PRINT "WHAT IS THE ID FOR THE INJECTION TO BE PROCESSED BY METHOD
*    ";T$[3,6];
0250 INPUT "?  ",D2$
0255 ON ERR THEN STOP
0260 IF LEN(D2$)=8 THEN GOTO 0300
0270 PRINT
0280 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0290 GOTO 0240
0300 LET D3$="GC",D2$

12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                      PROGRAM LISTING FOR GC09

12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
0310 ON ERR THEN GOTO 0330
0320 RENAME D3$,D3$
0330 ON ERR THEN STOP
0340 IF SYS(7)<>-48 THEN GOTO 0370
0350 DELAY =1
0360 GOTO 0310
0370 IF SYS(7)=-9 THEN GOTO 0410
0380 PRINT
0390 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0400 GOTO 0240
0410 ON ERR THEN GOTO 0450
0420 OPEN FILE[3,0],D3$,31
0430 ON ERR THEN STOP
0440 GOTO 0500
0450 ON ERR THEN STOP
0460 DELAY =1
0470 GOTO 0410
0480 REM   ---------------------------------------------------------------
0490 REM          CHECK DATA FILE USARILITY FLAG
0500 PRINT
0510 PRINT "PLEASE BE PATIENT."
0520 READ FILE[3,1],J
0530 IF J=1 THEN GOTO 0610
0540 PRINT
0550 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T DID NOT HAVE A TOTAL AREA."
0560 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T WAS IN THE WRONG FORMAT."
0570 CLOSE FILE[3]
0580 GOTO 0240
0590 REM   ---------------------------------------------------------------
0600 REM          DISPLAY ANY ERROR MESSAGES
0610 LET P9=2
0620 READ FILE[3,P9],V0$
0630 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0710
0640 PRINT
0650 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
0660 PRINT "     INJECTION ";D2$;":  ";V0$
0670 LET P9=P9+1
0680 GOTO 0620
0690 REM   ---------------------------------------------------------------
0700 REM          MATCH IDENTIFIER WITH CALIBRATION DATA

12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  3
                       PROGRAM LISTING FOR GC09

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0710 LET P9=P9+2
0720 READ FILE[3,P9],G$,H$,B,C
0730 IF EOF(3) THEN GOTO 1430
0740 REM    ------------------------------------
0750 REM      SKIP UNEXPLAINED PEAKS
0760 IF G$<>"XXXXXXXX" THEN GOTO 0820
0770 WRITE FILE[3,P9],G$,H$,B,C,-9999
0780 LET P9=P9+1
0790 GOTO 0720
0800 REM    ------------------------------------
0810 REM      LOCATE MATCHING IDENTIFIER IN METHOD FILE
0820 FOR I7=1 TO F
0830   READ FILE[4,3*I7-1],V$
0840   IF G$=V$ THEN GOTO 0960
0850 NEXT I7
0860 PRINT
0870 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*    AK WITH THE"
0880 PRINT "     IDENTIFIER '";G$;",' BUT METHOD ";T$[3,6];" DOES NOT
*    INCLUDE"
0890 PRINT "     THAT IDENTIFIER."
0900 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*    D."
0910 WRITE FILE[3,P9],G$,H$,B,C,-9999
0920 LET P9=P9+1
0930 GOTO 0720
0940 REM    ------------------------------------
0950 REM      CHECK WHETHER IDENTIFIER HAS BEEN CALIBRATED
0960 READ FILE[4,3*I7],D4$,I$,K,R1,R2,R3,J3
0965 LET F[I7]=1
0966 IF C=-9999 THEN GOTO 1410
0970 IF D4$<>"99/99/99" THEN GOTO 1080
0980 PRINT
0990 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*    AK WITH THE"
1000 PRINT "     IDENTIFIER '";G$;",' BUT THAT IDENTIFIER HAS NEVER BE
*    EN"
1010 PRINT "     CALIBRATED IN METHOD ";T$[3,6];"."
1020 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*    D."
1030 WRITE FILE[3,P9],G$,H$,B,C,-9999
1040 LET P9=P9+1

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  4
                       PROGRAM LISTING FOR GC09

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1050 GOTO 0720
1060 REM    -------------------------------------------------------------
1070 REM             CALCULATE CONCENTRATION USING REGRESSION EQUATION
1080 IF K=3 THEN GOTO 1160
1090 LET L=R1+R2*C
1100 IF K=2 THEN LET L=L+R3*C
1110 WRITE FILE[3,P9],G$,H$,B,C,L
1120 LET P9=P9+1
1130 GOTO 0720
1140 REM    -------------------------------------------------------------
1150 REM             CALCULATE CONCENTRATION USING INTERPOLATION
1160 LET I5=LEN(I$)/8
1170 MAT READ FILE[4,3*I7+1],G2
1180 IF I5=1 THEN GOTO 1200
1190 IF C>G2[2] THEN GOTO 1250
1200 LET M1=0
1210 LET M2=0
1220 LET M3=G2[1]
1230 LET M4=G2[2]
1240 GOTO 1390
1250 IF C<G2[2*I5] THEN GOTO 1310
1260 LET M1=G2[2*(I5-1)-1]
1270 LET M2=G2[2*(I5-1)]
1280 LET M3=G2[2*I5-1]
1290 LET M4=G2[2*I5]
1300 GOTO 1390
1310 LET I=2
1320 IF G2[2*I]>C THEN GOTO 1350
1330 LET I=I+1
1340 GOTO 1320
1350 LET M1=G2[2*(I-1)-1]
1360 LET M2=G2[2*(I-1)]
1370 LET M3=G2[2*I-1]
1380 LET M4=G2[2*I]
1390 LET L=((M3-M1)/(M4-M2))*(C-M2)+M1
1400 WRITE FILE[3,P9],G$,H$,B,C,L
1410 LET P9=P9+1
1420 GOTO 0720
1430 REM    -------------------------------------------------------------
1440 REM             ADD UNDETECTED COMPOUNDS TO DATA FILE
1450 FOR I=1 TO F
1460   IF F[I]=1 THEN GOTO 1500

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  5
                       PROGRAM LISTING FOR GC09

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
1470    READ FILE[4,3*I-1],G$
1475    IF G$="99999" THEN GOTO 1500
1480    WRITE FILE[3,P9],G$," ",-9999,-9999,-9999,-9999
1490    LET P9=P9+1
1500 NEXT I
1510 REM    ------------------------------------------------------------
1520 REM           CONTINUE INTO PROGRAM GC18
1530 NOESC
1540 CHAIN "GC12"

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  6
                        SYMBOL TABLE FOR GC09

SYMBOL  REFERENCES
------  ---------------------------------------------------------------
 0110   0080
 0112   0110
 0160   0100
 0180   0210
 0240   0190  0290  0400  0580
 0255   0245
 0300   0260
 0310   0360
 0330   0310
 0370   0340
 0410   0370  0470
 0450   0410
 0500   0440
 0610   0530
 0620   0680
 0710   0630
 0720   0790  0930  1050  1130  1420
 0820   0760
 0960   0840
 1080   0970
 1160   1080
 1200   1180
 1250   1190
 1310   1250
 1320   1340
 1350   1320
 1390   1240  1300
 1410   0966
 1430   0730
 1500   1460  1475
 B      0720  0770  0910  1030  1110  1400
 C      0720  0770  0910  0966  1030  1090  1100  1110  1190  1250
        1320  1390  1400
 D2$    0090  0250  0260  0280  0300  0390  0550  0560  0660  0870
        0990
 D3$    0090  0300  0320  0420
 D4$    0090  0960  0970
 F      0096  0160  0180  0200  0820  1450
 FL#3   0111  0420  0520  0570  0620  0720  0770  0910  1030  1110
        1400  1480
 FL#4   0170  0175  0176  0180  0830  0960  1170  1470
 F[     0095  0965  1460
 G$     0090  0720  0760  0770  0840  0880  0900  0910  1000  1020
        1030  1110  1400  1470  1475  1480
 G2     1170
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  7
                       SYMBOL TABLE FOR GC09

SYMBOL   REFERENCES
------  ------------------------------------------------------------
 G2[    0090  1190  1220  1230  1250  1260  1270  1280  1290  1320
        1350  1360  1370  1380
 H$     0090  0720  0770  0910  1030  1110  1400
 I      1310  1320  1330  1350  1360  1370  1380  1450  1460  1470
        1500
 I$     0090  0960  1160
 I5     1160  1180  1250  1260  1270  1280  1290
 I7     0820  0830  0850  0960  0965  1170
 J      0520  0530  0550  0560
 J3     0960
 K      0960  1080  1100
 L      1090  1100  1110  1390  1400
 M1     1200  1260  1350  1390
 M2     1210  1270  1360  1390
 M3     1220  1280  1370  1390
 M4     1230  1290  1380  1390
 P9     0610  0620  0670  0710  0720  0770  0780  0910  0920  1030
        1040  1110  1120  1400  1410  1480  1490
 R1     0960  1090
 R2     0960  1090
 R3     0960  1100
 T$     0090  0170  0176  0248  0880  1010
 V$     0090  0180  0830  0840
 VO$    0090  0620  0630  0660
```

SECTION 12

PROGRAM GC10 - LIQUID/LIQUID EXTRACTION CONCENTRATION CALCULATION

GC10 is the program which calculates concentrations of samples prepared by the liquid/liquid extraction method. It is essentially the same as program GC09. The only difference is that this program asks the user for the volume of the injection, the volume of the extract, and the volume of the water extracted. Using the calibration equations, this program calculates the mass in nanograms of each compound. It multiplies this mass by the volume of the extract (in milliliters) and divides by the product of the volume of the injection (in microliters) and the volume of the water extracted (in liters). This produces the concentration in micrograms per liter.

There are three additional symbols used in GC10. They are:

Q	the volume of the injection
R	the volume of the extract
S	the volume of the water extracted

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                        PROGRAM LISTING FOR GC10

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                  +
0030 REM   +   PROGRAM GC10, LIQUID/LIQUID EXTRACTION PROCESSING     +
0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 19, 1979                +
0045 REM   +   MOST RECENT REVISION:  APRIL 2, 1979                  +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 0110
0090 DIM D2$[8],D3$[10],D4$[8],G$[8],G2[30],H$[2],I$[160],T$[6],V$[8],
*    VO$[20]
0095 DIM F[60]
0096 MAT F=ZER
0100 GOTO 0160
0110 ON ERR THEN GOTO 0112
0111 CLOSE FILE[3]
0112 ON ERR THEN STOP
0120 NOESC
0130 CHAIN "GC00"
0140 REM      --------------------------------------------------------
0150 REM                  COUNT IDENTIFIERS IN METHOD FILE
0160 LET F=0
0170 READ FILE[4,1],T$
0175 CLOSE FILE[4]
0176 OPEN FILE[4,0],T$,200
0180 READ FILE[4,3*(F+1)-1],V$
0190 IF EOF(4) THEN GOTO 0240
0200 LET F=F+1
0210 GOTO 0180
0220 REM      --------------------------------------------------------
0230 REM                  OPEN DATA FILE
0240 PRINT
0245 ON ERR THEN GOTO 0255
0248 PRINT "WHAT IS THE ID FOR THE INJECTION TO BE PROCESSED BY METHOD
*     ";T$[3,6];
0250 INPUT "?  ",D2$
0255 ON ERR THEN STOP
0260 IF LEN(D2$)=8 THEN GOTO 0300
0270 PRINT
0280 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0290 GOTO 0240
0300 LET D3$="GC",D2$

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                        PROGRAM LISTING FOR GC10

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0310 ON ERR THEN GOTO 0330
0320 RENAME D3$,D3$
0330 ON ERR THEN STOP
0340 IF SYS(7)<>-48 THEN GOTO 0370
0350 DELAY =1
0360 GOTO 0310
0370 IF SYS(7)=-9 THEN GOTO 0410
0380 PRINT
0390 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0400 GOTO 0240
0410 ON ERR THEN GOTO 0450
0420 OPEN FILE[3,0],D3$,31
0430 ON ERR THEN STOP
0440 GOTO 0520
0450 ON ERR THEN STOP
0460 DELAY =1
0470 GOTO 0410
0480 REM      --------------------------------------------------------
0490 REM                  CHECK DATA FILE USABILITY FLAG
0520 READ FILE[3,1],J
0530 IF J=1 THEN GOTO 0610
0540 PRINT
0550 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T DID NOT HAVE A TOTAL AREA."
0560 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T WAS IN THE WRONG FORMAT."
0570 CLOSE FILE[3]
0580 GOTO 0240
0590 REM      --------------------------------------------------------
0600 REM                  DISPLAY ANY ERROR MESSAGES
0610 LET P9=2
0620 READ FILE[3,P9],VO$
0630 IF VO$[1,7]<>"MESSAGE" THEN GOTO 0702
0640 PRINT
0650 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
0660 PRINT "     INJECTION ";D2$;":  ";VO$
0670 LET P9=P9+1
0680 GOTO 0620
0690 REM      --------------------------------------------------------
0700 REM                  MATCH IDENTIFIER WITH CALIBRATION DATA
0702 INPUT "     VOLUME OF THE INJECTION, IN MICROLITERS?  ",Q
0704 INPUT "     VOLUME OF THE EXTRACT, IN MILLILITERS?  ",R

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  3
                        PROGRAM LISTING FOR GC10

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0706 INPUT "     VOLUME OF THE WATER EXTRACTED, IN LITERS?  ",S
0708 PRINT
0709 PRINT "PLEASE BE PATIENT."
0710 LET P9=P9+2
0720 READ FILE[3,P9],G$,H$,B,C
0730 IF EOF(3) THEN GOTO 1430
0740 REM   ------------------------------------------
0750 REM     SKIP UNEXPLAINED PEAKS
0760 IF G$<>"XXXXXXXX" THEN GOTO 0820
0770 WRITE FILE[3,P9],G$,H$,B,C,-9999
0780 LET P9=P9+1
0790 GOTO 0720
0800 REM   ------------------------------------------
0810 REM     LOCATE MATCHING IDENTIFIER IN METHOD FILE
0820 FOR I7=1 TO F
0830   READ FILE[4,3*I7-1],V$
0840   IF G$=V$ THEN GOTO 0960
0850 NEXT I7
0860 PRINT
0870 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*     AK WITH THE"
0880 PRINT "     IDENTIFIER '";G$;",' BUT METHOD ";T$[3,6];" DOES NOT
*     INCLUDE"
0890 PRINT "     THAT IDENTIFIER."
0900 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*     D."
0910 WRITE FILE[3,P9],G$,H$,B,C,-9999
0920 LET P9=P9+1
0930 GOTO 0720
0940 REM   ------------------------------------------
0950 REM     CHECK WHETHER IDENTIFIER HAS BEEN CALIBRATED
0960 READ FILE[4,3*I7],D4$,I$,K,R1,R2,R3,J3
0965 LET F[I7]=1
0966 IF C=-9999 THEN GOTO 1410
0970 IF D4$<>"99/99/99" THEN GOTO 1080
0980 PRINT
0990 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*     AK WITH THE"
1000 PRINT "     IDENTIFIER '";G$;",' BUT THAT IDENTIFIER HAS NEVER BE
*     EN"
1010 PRINT "     CALIBRATED IN METHOD ";T$[3,6];"."
1020 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*     D."

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  4
                        PROGRAM LISTING FOR GC10

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1030 WRITE FILE[3,P9],G$,H$,B,C,-9999
1040 LET P9=P9+1
1050 GOTO 0720
1060 REM   -------------------------------------------------------------
1070 REM             CALCULATE CONCENTRATION USING REGRESSION EQUATION
1080 IF K=3 THEN GOTO 1160
1090 LET L=R1+R2*C
1100 IF K=2 THEN LET L=L+R3*C
1105 LET L=(L*R)/(Q*S)
1110 WRITE FILE[3,P9],G$,H$,B,C,L
1120 LET P9=P9+1
1130 GOTO 0720
1140 REM   -------------------------------------------------------------
1150 REM             CALCULATE CONCENTRATION USING INTERPOLATION
1160 LET I5=LEN(I$)/8
1170 MAT READ FILE[4,3*I7+1],G2
1180 IF I5=1 THEN GOTO 1200
1190 IF C>G2[2] THEN GOTO 1250
1200 LET M1=0
1210 LET M2=0
1220 LET M3=G2[1]
1230 LET M4=G2[2]
1240 GOTO 1390
1250 IF C<G2[2*I5] THEN GOTO 1310
1260 LET M1=G2[2*(I5-1)-1]
1270 LET M2=G2[2*(I5-1)]
1280 LET M3=G2[2*I5-1]
1290 LET M4=G2[2*I5]
1300 GOTO 1390
1310 LET I=2
1320 IF G2[2*I]>C THEN GOTO 1350
1330 LET I=I+1
1340 GOTO 1320
1350 LET M1=G2[2*(I-1)-1]
1360 LET M2=G2[2*(I-1)]
1370 LET M3=G2[2*I-1]
1380 LET M4=G2[2*I]
1390 LET L=((M3-M1)/(M4-M2))*(C-M2)+M1
1395 LET L=(L*R)/(Q*S)
1400 WRITE FILE[3,P9],G$,H$,B,C,L
1410 LET P9=P9+1
1420 GOTO 0720

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  5
                    PROGRAM LISTING FOR GC10

 12345678911234567892123456789312345678941234567895123456789612345678970
         0         0         0         0         0         0         0
 1430 REM  ----------------------------------------------------------------
 1440 REM          ADD UNDETECTED COMPOUNDS TO DATA FILE
 1450 FOR I=1 TO F
 1460   IF F[I]=1 THEN GOTO 1500
 1470   READ FILE[4,3*I-1],G$
 1475   IF G$="99999" THEN GOTO 1500
 1480   WRITE FILE[3,P9],G$," ",-9999,-9999,-9999,-9999
 1490   LET P9=P9+1
 1500 NEXT I
 1510 REM  ----------------------------------------------------------------
 1520 REM          CONTINUE INTO PROGRAM GC18
 1530 NOESC
 1540 CHAIN "GC12"






















12345678911234567892123456789312345678941234567895123456789612345678970
        0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  6
                      SYMBOL TABLE FOR GC10

SYMBOL   REFERENCES
------   ------------------------------------------------------------
 0110    0080
 0112    0110
 0160    0100
 0180    0210
 0240    0190  0290  0400  0580
 0255    0245
 0300    0260
 0310    0360
 0330    0310
 0370    0340
 0410    0370  0470
 0450    0410
 0520    0440
 0610    0530
 0620    0680
 0702    0630
 0720    0790  0930  1050  1130  1420
 0820    0760
 0960    0840
 1080    0970
 1160    1080
 1200    1180
 1250    1190
 1310    1250
 1320    1340
 1350    1320
 1390    1240  1300
 1410    0966
 1430    0730
 1500    1460  1475
 B       0720  0770  0910  1030  1110  1400
 C       0720  0770  0910  0966  1030  1090  1100  1110  1190  1250
         1320  1390  1400
 D2$     0090  0250  0260  0280  0300  0390  0550  0560  0660  0870
         0990
 D3$     0090  0300  0320  0420
 D4$     0090  0960  0970
 F       0096  0160  0180  0200  0820  1450
 FL#3    0111  0420  0520  0570  0620  0720  0770  0910  1030  1110
         1400  1480
 FL#4    0170  0175  0176  0180  0830  0960  1170  1470
 F[      0095  0965  1460
 G$      0090  0720  0760  0770  0840  0880  0900  0910  1000  1020
         1030  1110  1400  1470  1475  1480
 G2      1170
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                          PAGE  7
                         SYMBOL TABLE FOR GC10

SYMBOL    REFERENCES
------  ------------------------------------------------------------------
 G2[    0090  1190  1220  1230  1250  1260  1270  1280  1290  1320
        1350  1360  1370  1380
 H$     0090  0720  0770  0910  1030  1110  1400
 I      1310  1320  1330  1350  1360  1370  1380  1450  1460  1470
        1500
 I$     0090  0960  1160
 I5     1160  1180  1250  1260  1270  1280  1290
 I7     0820  0830  0850  0960  0965  1170
 J      0520  0530  0550  0560
 J3     0960
 K      0960  1080  1100
 L      1090  1100  1105  1110  1390  1395  1400
 M1     1200  1260  1350  1390
 M2     1210  1270  1360  1390
 M3     1220  1280  1370  1390
 M4     1230  1290  1380  1390
 P9     0610  0620  0670  0710  0720  0770  0780  0910  0920  1030
        1040  1110  1120  1400  1410  1480  1490
 Q      0702  1105  1395
 R      0704  1105  1395
 R1     0960  1090
 R2     0960  1090
 R3     0960  1100
 S      0706  1105  1395
 T$     0090  0170  0176  0248  0880  1010
 V$     0090  0180  0830  0840
 VO$    0090  0620  0630  0660
```

SECTION 13

PROGRAM GC11 - DIRECT AQUEOUS INJECTION CONCENTRATION CALCULATION

GC11 is the program which calculates concentrations of samples prepared by the direct aqueous injection method. It is essentially the same as program GC09. The only difference is that this program asks the user for the volume of the injection. Using the calibration equations, this program calculates the mass in nanograms of each compound. It divides this mass by the injection volume (in microliters) and then divides by 1000 to produce the concentration in micrograms per liter.

There is one additional symbol used in GC11. It is Q, the volume of the injection.

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                       PROGRAM LISTING FOR GC11

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
 0030 REM   +   PROGRAM GC11, DIRECT AQUEOUS INJECTION PROCESSING       +
 0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 20, 1979                  +
 0045 REM   +   MOST RECENT REVISION:  APRIL 2, 1979                    +
 0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0060 REM
 0070 ESC
 0080 ON ESC THEN GOTO 0110
 0090 DIM D2$[8],D3$[10],D4$[8],G$[8],G2[30],H$[2],I$[160],T$[6],V$[8],
*     V0$[20]
 0095 DIM F[60]
 0096 MAT F=ZER
 0100 GOTO 0160
 0110 ON ERR THEN GOTO 0112
 0111 CLOSE FILE[3]
 0112 ON ERR THEN STOP
 0120 NOESC
 0130 CHAIN "GC00"
 0140 REM   -----------------------------------------------------------
 0150 REM             COUNT IDENTIFIERS IN METHOD FILE
 0160 LET F=0
 0170 READ FILE[4,1],T$
 0175 CLOSE FILE[4]
 0176 OPEN FILE[4,0],T$,200
 0180 READ FILE[4,3*(F+1)-1],V$
 0190 IF EOF(4) THEN GOTO 0240
 0200 LET F=F+1
 0210 GOTO 0180
 0220 REM   -----------------------------------------------------------
 0230 REM             OPEN DATA FILE
 0240 PRINT
 0245 ON ERR THEN GOTO 0255
 0248 PRINT "WHAT IS THE ID FOR THE INJECTION TO BE PROCESSED BY METHOD
*       ";T$[3,6];
 0250 INPUT "?  ",D2$
 0255 ON ERR THEN STOP
 0260 IF LEN(D2$)=8 THEN GOTO 0300
 0270 PRINT
 0280 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
 0290 GOTO 0240
 0300 LET D3$="GC",D2$

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                       PROGRAM LISTING FOR GC11

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0310 ON ERR THEN GOTO 0330
 0320 RENAME D3$,D3$
 0330 ON ERR THEN STOP
 0340 IF SYS(7)<>-48 THEN GOTO 0370
 0350 DELAY =1
 0360 GOTO 0310
 0370 IF SYS(7)=-9 THEN GOTO 0410
 0380 PRINT
 0390 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
 0400 GOTO 0240
 0410 ON ERR THEN GOTO 0450
 0420 OPEN FILE[3,0],D3$,31
 0430 ON ERR THEN STOP
 0440 GOTO 0520
 0450 ON ERR THEN STOP
 0460 DELAY =1
 0470 GOTO 0410
 0480 REM   -----------------------------------------------------------
 0490 REM             CHECK DATA FILE USABILITY FLAG
 0520 READ FILE[3,1],J
 0530 IF J=1 THEN GOTO 0610
 0540 PRINT
 0550 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*     T DID NOT HAVE A TOTAL AREA."
 0560 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*     T WAS IN THE WRONG FORMAT."
 0570 CLOSE FILE[3]
 0580 GOTO 0240
 0590 REM   -----------------------------------------------------------
 0600 REM             DISPLAY ANY ERROR MESSAGES
 0610 LET P9=2
 0620 READ FILE[3,P9],V0$
 0630 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0702
 0640 PRINT
 0650 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
 0660 PRINT "      INJECTION ";D2$;":  ";V0$
 0670 LET P9=P9+1
 0680 GOTO 0620
 0690 REM   -----------------------------------------------------------
 0700 REM             MATCH IDENTIFIER WITH CALIBRATION DATA
 0702 INPUT "      VOLUME OF THE INJECTION, IN MICROLITERS?  ",Q
 0708 PRINT

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                          PAGE  3
                        PROGRAM LISTING FOR GC11

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0709 PRINT "PLEASE BE PATIENT."
 0710 LET P9=P9+2
 0720 READ FILE[3,P9],G$,H$,B,C
 0730 IF EOF(3) THEN GOTO 1430
 0740 REM  ------------------------------------
 0750 REM     SKIP UNEXPLAINED PEAKS
 0760 IF G$<>"XXXXXXXX" THEN GOTO 0820
 0770 WRITE FILE[3,P9],G$,H$,B,C,-9999
 0780 LET P9=P9+1
 0790 GOTO 0720
 0800 REM  ------------------------------------
 0810 REM     LOCATE MATCHING IDENTIFIER IN METHOD FILE
 0820 FOR I7=1 TO F
 0830   READ FILE[4,3*I7-1],V$
 0840   IF G$=V$ THEN GOTO 0960
 0850 NEXT I7
 0860 PRINT
 0870 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*     AK WITH THE"
 0880 PRINT "     IDENTIFIER '";G$;",' BUT METHOD ";T$[3,6];" DOES NOT
*     INCLUDE"
 0890 PRINT "     THAT IDENTIFIER."
 0900 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*     D."
 0910 WRITE FILE[3,P9],G$,H$,B,C,-9999
 0920 LET P9=P9+1
 0930 GOTO 0720
 0940 REM  ------------------------------------
 0950 REM     CHECK WHETHER IDENTIFIER HAS BEEN CALIBRATED
 0960 READ FILE[4,3*I7],D4$,I$,K,R1,R2,R3,J3
 0965 LET F[I7]=1
 0966 IF C=-9999 THEN GOTO 1410
 0970 IF D4$<>"99/99/99" THEN GOTO 1080
 0980 PRINT
 0990 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*     AK WITH THE"
 1000 PRINT "     IDENTIFIER '";G$;",' BUT THAT IDENTIFIER HAS NEVER BE
*     EN"
 1010 PRINT "     CALIBRATED IN METHOD ";T$[3,6];"."
 1020 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*     D."
 1030 WRITE FILE[3,P9],G$,H$,B,C,-9999

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                          PAGE  4
                        PROGRAM LISTING FOR GC11

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 1040 LET P9=P9+1
 1050 GOTO 0720
 1060 REM  ----------------------------------------------------------
 1070 REM          CALCULATE CONCENTRATION USING REGRESSION EQUATION
 1080 IF K=3 THEN GOTO 1160
 1090 LET L=R1+R2*C
 1100 IF K=2 THEN LET L=L+R3*C
 1105 LET L=L/Q/1000
 1110 WRITE FILE[3,P9],G$,H$,B,C,L
 1120 LET P9=P9+1
 1130 GOTO 0720
 1140 REM  ----------------------------------------------------------
 1150 REM          CALCULATE CONCENTRATION USING INTERPOLATION
 1160 LET I5=LEN(I$)/8
 1170 MAT READ FILE[4,3*I7+1],G2
 1180 IF I5=1 THEN GOTO 1200
 1190 IF C>G2[2] THEN GOTO 1250
 1200 LET M1=0
 1210 LET M2=0
 1220 LET M3=G2[1]
 1230 LET M4=G2[2]
 1240 GOTO 1390
 1250 IF C<G2[2*I5] THEN GOTO 1310
 1260 LET M1=G2[2*(I5-1)-1]
 1270 LET M2=G2[2*(I5-1)]
 1280 LET M3=G2[2*I5-1]
 1290 LET M4=G2[2*I5]
 1300 GOTO 1390
 1310 LET I=2
 1320 IF G2[2*I]>C THEN GOTO 1350
 1330 LET I=I+1
 1340 GOTO 1320
 1350 LET M1=G2[2*(I-1)-1]
 1360 LET M2=G2[2*(I-1)]
 1370 LET M3=G2[2*I-1]
 1380 LET M4=G2[2*I]
 1390 LET L=((M3-M1)/(M4-M2))*(C-M2)+M1
 1395 LET L=L/Q/1000
 1400 WRITE FILE[3,P9],G$,H$,B,C,L
 1410 LET P9=P9+1
 1420 GOTO 0720
 1430 REM  ----------------------------------------------------------

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  5
                     PROGRAM LISTING FOR GC11

 1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
 1440 REM           ADD UNDETECTED COMPOUNDS TO DATA FILE
 1450 FOR I=1 TO F
 1460   IF F[I]=1 THEN GOTO 1500
 1470   READ FILE[4,3*I-1],G$
 1475   IF G$="99999" THEN GOTO 1500
 1480   WRITE FILE[3,P9],G$," ",-9999,-9999,-9999,-9999
 1490   LET P9=P9+1
 1500 NEXT I
 1510 REM   ----------------------------------------------------------
 1520 REM           CONTINUE INTO PROGRAM GC18
 1530 NOESC
 1540 CHAIN "GC12"










 1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  6
                          SYMBOL TABLE FOR GC11

SYMBOL    REFERENCES
------    ------------------------------------------------------------
 0110   0080
 0112   0110
 0160   0100
 0180   0210
 0240   0190  0290  0400  0580
 0255   0245
 0300   0260
 0310   0360
 0330   0310
 0370   0340
 0410   0370  0470
 0450   0410
 0520   0440
 0610   0530
 0620   0680
 0702   0630
 0720   0790  0930  1050  1130  1420
 0820   0760
 0960   0840
 1080   0970
 1160   1080
 1200   1180
 1250   1190
 1310   1250
 1320   1340
 1350   1320
 1390   1240  1300
 1410   0966
 1430   0730
 1500   1460  1475
 B      0720  0770  0910  1030  1110  1400
 C      0720  0770  0910  0966  1030  1090  1100  1110  1190  1250
        1320  1390  1400
 D2$    0090  0250  0260  0280  0300  0390  0550  0560  0660  0870
        0990
 D3$    0090  0300  0320  0420
 D4$    0090  0960  0970
 F      0096  0160  0180  0200  0820  1450
 FL#3   0111  0420  0520  0570  0620  0720  0770  0910  1030  1110
        1400  1480
 FL#4   0170  0175  0176  0180  0830  0960  1170  1470
 F[     0095  0965  1460
 G$     0090  0720  0760  0770  0840  0880  0900  0910  1000  1020
        1030  1110  1400  1470  1475  1480
 G2     1170
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE  7
                       SYMBOL TABLE FOR GC11

SYMBOL   REFERENCES
------  -------------------------------------------------------------
 G2[    0090  1190  1220  1230  1250  1260  1270  1280  1290  1320
        1350  1360  1370  1380
 H$     0090  0720  0770  0910  1030  1110  1400
 I      1310  1320  1330  1350  1360  1370  1380  1450  1460  1470
        1500
 I$     0090  0960  1160
 I5     1160  1180  1250  1260  1270  1280  1290
 I7     0820  0830  0850  0960  0965  1170
 J      0520  0530  0550  0560
 J3     0960
 K      0960  1080  1100
 L      1090  1100  1105  1110  1390  1395  1400
 M1     1200  1260  1350  1390
 M2     1210  1270  1360  1390
 M3     1220  1280  1370  1390
 M4     1230  1290  1380  1390
 P9     0610  0620  0670  0710  0720  0770  0780  0910  0920  1030
        1040  1110  1120  1400  1410  1480  1490
 Q      0702  1105  1395
 R1     0960  1090
 R2     0960  1090
 R3     0960  1100
 T$     0090  0170  0176  0248  0880  1010
 V$     0090  0180  0830  0840
 VO$    0090  0620  0630  0660
```

SECTION 14

PROGRAM GC12 - RETENTION TIME CALCULATION

GC12 is the program which calculates relative retention times or capacity ratios. It is entered by chaining from any of the concentration calculation programs (GC08, GC09, GC10, or GC11).

As the program begins, the method file and the injection data file are already open, although at several places in the program, the data file is closed and reopened to set the EOF function for that file back to zero.

The program reads from the method file the flag for the type of retention time calculations and either the relative retention time reference identifier or the capacity ratio dead time. It then branches to the appropriate section of code.

To calculate relative retention times, this program first searches the data file for the identifier of the relative retention time reference peak. If that identifier does not appear in the data file, the program informs the user that relative retention times cannot be calculated, and puts -9999 into the injection data file as the relative retention time of every peak. Conversely, if the program does find the relative retention time reference peak in the data file, it uses its retention time to calculate the relative retention time of every peak in the data file and places those calculated values into the data file. The formula for relative retention time is:

$$\text{Rel. Retn. Time} = \frac{\text{Retn. Time}}{\text{Retn. Time of Reference}} \cdot 100.$$

The formula for capacity ratio is:

$$\text{Capacity Ratio} = \frac{\text{Retn. Time}}{\text{Dead Volume Time}} - 1.$$

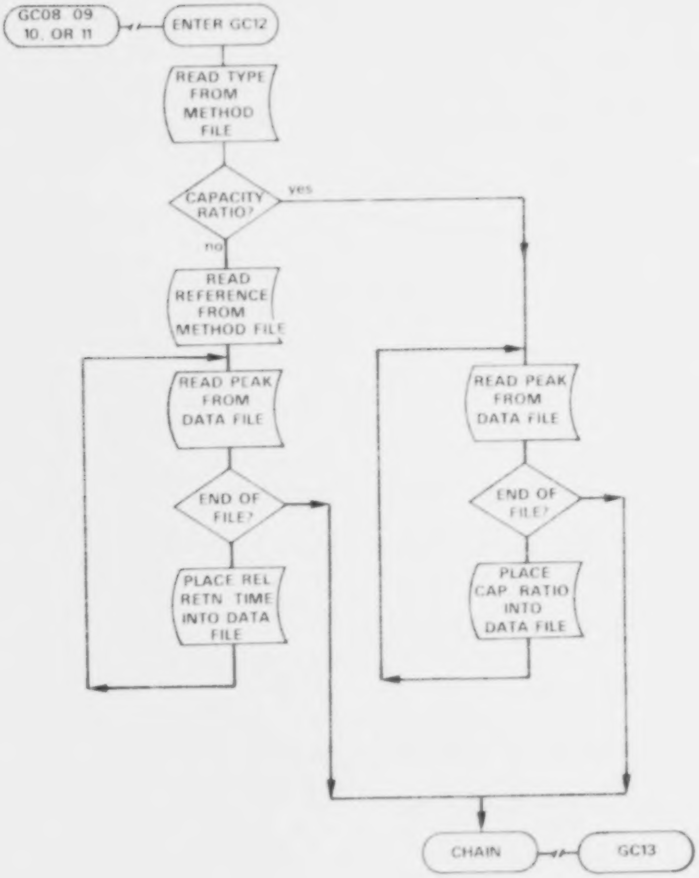

GC08 09 10, OR 11
ENTER GC12
READ TYPE FROM METHOD FILE
CAPACITY RATIO?
yes
no
READ REFERENCE FROM METHOD FILE
READ PEAK FROM DATA FILE
END OF FILE?
PLACE REL RETN TIME INTO DATA FILE
READ PEAK FROM DATA FILE
END OF FILE?
PLACE CAP RATIO INTO DATA FILE
CHAIN
GC13

Figure 10. Flowchart of Program GC12.

TABLE 8. SYMBOL DEFINITIONS FOR PROGRAM GC12

B	the absolute retention time of a peak
C	the area of a peak
D3$	the name of the data file
G$	an identifier from a data file
H$	the peak type
I2	the data file record number of the peak being processed
J	the data file useability flag
L	the calculated concentration
L2	the calculated relative retention time or capacity ratio
N$	the relative retention time reference peak or the capacity ratio dead time as a string
N1	the type of method
N2	the type of retention time calculations N2=1 relative retention time N2=2 capacity ratio
N3	retention time of a peak
N4	capacity ratio dead time
P9	the record number of the first peak in the data file
T$	the name of the method file
U$	the name of the user
VO$	a MESSAGE from the data file

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                          PROGRAM LISTING FOR GC12

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                     +
0030 REM   +   PROGRAM GC12, RETENTION TIME CALCULATIONS                +
0040 REM   +   BY:  J. KOPKE (SWORCC), FEBRUARY 14, 1979                +
0045 REM   +   MOST RECENT REVISION:  MARCH 21, 1979                    +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 0100
0090 GOTO 0130
0100 ON ERR THEN GOTO 0102
0101 CLOSE FILE[3]
0102 ON ERR THEN STOP
0110 NOESC
0120 CHAIN "GC00"
0130 DIM D3$[10],G$[8],H$[2],N$[8],T$[6],U$[30],V0$[20]
0140 REM   ----------------------------------------------------------------
0150 REM          DETERMINE TYPE; FIND WHERE TO START
0160 READ FILE[3,1],J,D3$
0170 READ FILE[4,1],T$,U$,N1,N2,N$
0180 LET P9=2
0190 READ FILE[3,P9],V0$
0200 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0230
0210 LET P9=P9+1
0220 GOTO 0190
0230 LET P9=P9+2
0240 IF N2=2 THEN GOTO 0640
0250 REM   ----------------------------------------------------------------
0260 RFM          RELATIVE RETENTION TIME
0270 LET I2=P9
0280 CLOSE FILE[3]
0290 OPEN FILE[3,0],D3$,31
0300 READ FILE[3,I2],G$,H$,B,C,L
0310 IF EOF(3) THEN GOTO 0370
0320 IF G$=N$ THEN GOTO 0520
0330 LET I2=I2+1
0340 GOTO 0300
0350 REM   ----------------------------------------
0360 REM      CANNOT CALCULATE RELATIVE RETENTION TIMES
0370 PRINT
0380 PRINT "<7><7>METHOD ";T$[3,6];" SPECIFIES THAT THE REFERENCE PEAK
*     FOR RELATIVE"

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                          PROGRAM LISTING FOR GC12

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0390 PRINT "     RFTENTION TIME IS ";N$;", BUT THE REPORT FOR INJECTIO
*    N ";D3$[3]
0400 PRINT "     DOES NOT INCLUDE A PEAK WITH THAT IDENTIFIER."
0410 PRINT "THEREFORE, NO RELATIVE RETENTION TIMES CAN BE CALCULATED."
0420 LET I2=P9
0430 CLOSE FILE[3]
0440 OPEN FILE[3,0],D3$,31
0450 READ FILE[3,I2],G$,H$,B,C,L
0460 IF EOF(3) THEN GOTO 0760
0470 WRITE FILE[3,I2],G$,H$,B,C,L,-9999
0480 LET I2=I2+1
0490 GOTO 0450
0500 REM   ------------------------------------
0510 REM     PUT RELATIVE RETENTION TIME IN DATA FILE
0520 LET N3=B
0530 LET I2=P9
0540 CLOSE FILE[3]
0550 OPEN FILE[3,0],D3$,31
0560 READ FILE[3,I2],G$,H$,B,C,L
0570 IF EOF(3) THEN GOTO 0760
0580 LET L2=(B/N3)*100
0590 WRITE FILE[3,I2],G$,H$,B,C,L,L2
0600 LET I2=I2+1
0610 GOTO 0560
0620 REM   ----------------------------------------------------------------
0630 REM          CAPACITY RATIO
0640 LET N4=VAL(N$)
0650 LET I2=P9
0660 CLOSE FILE[3]
0670 OPEN FILE[3,0],D3$,31
0680 READ FILE[3,I2],G$,H$,B,C,L
0690 IF EOF(3) THEN GOTO 0760
0700 LET L2=(B/N4)-1
0710 WRITE FILE[3,I2],G$,H$,B,C,L,L2
0720 LET I2=I2+1
0730 GOTO 0680
0740 REM   ----------------------------------------------------------------
0750 REM          FLAG DATA FILE AS BEING PROCESSED
0760 READ FILE[3,1],J,D3$
0770 WRITE FILE[3,1],J,D3$,1
0780 REM   ----------------------------------------------------------------
0790 REM          CONTINUE INTO PROGRAM GC19

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE  3
                      PROGRAM LISTING FOR GC12

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0800 NOESC
0810 CHAIN "GC13"




















1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE  4
                      SYMBOL TABLE FOR GC12

SYMBOL    REFFRENCES
------  ----------------------------------------------------------------
 0100   0080
 0102   0100
 0130   0090
 0190   0220
 0230   0200
 0300   0340
 0370   0310
 0450   0490
 0520   0320
 0560   0610
 0640   0240
 0680   0730
 0760   0460  0570  0690
 B      0300  0450  0470  0520  0560  0580  0590  0680  0700  0710
 C      0300  0450  0470  0560  0590  0680  0710
 D3$    0130  0160  0290  0390  0440  0550  0670  0760  0770
 FL#3   0101  0160  0190  0280  0290  0300  0430  0440  0450  0470
        0540  0550  0560  0590  0660  0670  0680  0710  0760  0770
 FL#4   0170
 G$     0130  0300  0320  0450  0470  0560  0590  0680  0710
 H$     0130  0300  0450  0470  0560  0590  0680  0710
 I2     0270  0300  0330  0420  0450  0470  0480  0530  0560  0590
        0600  0650  0680  0710  0720
 J      0160  0760  0770
 L      0300  0450  0470  0560  0590  0680  0710
 L2     0580  0590  0700  0710
 N$     0130  0170  0320  0390  0640
 N1     0170
 N2     0170  0240
 N3     0520  0580
 N4     0640  0700
 P9     0180  0190  0210  0230  0270  0420  0530  0650
 T$     0130  0170  0380
 U$     0130  0170
 V0$    0130  0190  0200
```

SECTION 15

PROGRAM GC13 - COMPOUND IDENTIFICATION AND DATA PROCESSING REPORT

GC13 is the program which prints the injection data processing report. In doing so, it must also locate the true chemical name and CAS Registry number for each of the named peaks. This program is entered by chaining from the retention time calculation program, GC12. If the escape key is pressed during the execution of GC13, the program chains back to the master control program, GC00.

As GC13 begins, both the injection data file and the method file are already open, although in the program both of these files are closed and promptly reopened to set the EOF functions for them back to zero. This program also opens a temporary formatted output file where it places the lines of the report as they are generated. This avoids having the program monopolize the lineprinter while it searches other files for data.

The first section of this program fills the temporary formatted output file. A record of information is read from the data file, and if that record represents an unexplained peak, this program uses "UNEXPLAINED PEAK" as the name of the compound and a null string as the CAS number. If the record from the data file is a named peak, this program uses the compound name(s) and CAS number(s) from the method file. If there is no matching identifier in the method file, the program uses the string "(identifier - NOT IN METHOD XXXX)" as the name of the compound and a null string as the CAS number. The rest of the numeric items are also written into the temporary file, although if the relative retention time is -9999 (indicating that the item could not be calculated), the corresponding space is left blank.

After all of the records of the data file have been transformed into lines in the temporary file, the program copies the temporary file to the lineprinter. Headings are printed and paging occurs.

When the entire temporary file has been transferred to the lineprinter, all files except the method file are closed and the temporary file is deleted. The program then asks if the user wants to process another injection. If the answer is no, this program disables the escape key and chains back to GC00. If the answer is yes, this program disables the escape key and chains back to the appropriate concentration calculation program, as determined by the type of method flag in the method file.

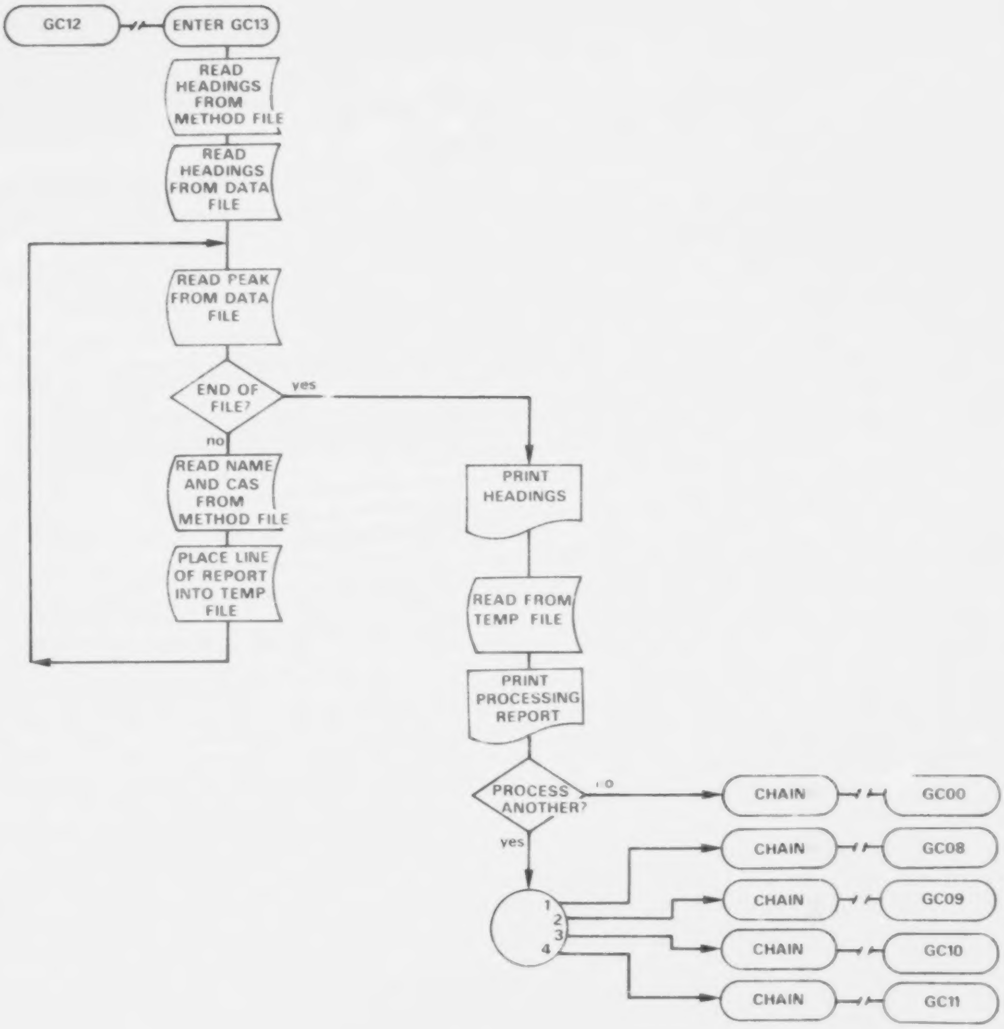

GC12
ENTER GC13
READ HEADINGS FROM METHOD FILE
READ HEADINGS FROM DATA FILE
READ PEAK FROM DATA FILE
END OF FILE?
yes
no
READ NAME AND CAS FROM METHOD FILE
PLACE LINE OF REPORT INTO TEMP FILE
PRINT HEADINGS
READ FROM TEMP FILE
PRINT PROCESSING REPORT
PROCESS ANOTHER?
no
yes
1
2
3
4
CHAIN
GC00
CHAIN
GC08
CHAIN
GC09
CHAIN
GC10
CHAIN
GC11

Figure 11. Flowchart of Program GC13.

TABLE 9. SYMBOL DEFINITIONS FOR PROGRAM GC13

B	the absolute retention time of a peak
C	the area of a peak
D3$	the name of the data file
F$	the report title
G$	an identifier from a data file
H$	the peak type
I	the control variable for a loop
I5	the number of identifiers in the method file
I6	the data file position of the peak being processed
I7	the page number of the printed report
J	the data file useability flag
L	the calculated concentration
L2	the calculated relative retention time or capacity ratio
N1	the type of method N1=1 internal standards N1=2 purge and trap N1=3 liquid/liquid extraction N1=4 direct aqueous injection
N2	the type of retention time calculations N2=1 relative retention time N2=2 capacity ratio
P9	the data file record number for the report title
Q$	the name of the temporary formatted output file
Q5$	a format for a PRINT USING statement

TABLE 9. (Continued)

Q6$	a format for a PRINT USING statement
Q7$	the type of method
Q8$	a line being transferred from the temporary formatted output file to the lineprinter
Q9$	the carriage return for Q8$
T$	the name of the method file
U$	the name of the user
V$	an identifier from the method file
V0$	a MESSAGE from the data file
V1$	the name of the first compound associated with an identifier
V2$	the CAS number for V1$
V3$	the name of the second compound associated with an identifier
V4$	the CAS number for V3$
V5$	the name of the third compound associated with an identifier
V6$	the CAS number for V5$
X$	the user's answer to a Y or N question

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                         PAGE  1
                        PROGRAM LISTING FOR GC13

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                     +
 0030 REM   +   PROGRAM GC13, COMPOUND IDENTIFICATION AND REPORT         +
 0040 REM   +   BY:  J. KOPKE (SWORCC), FEBRUARY 15, 1979                +
 0045 REM   +   MOST RECENT REVISION:  APRIL 12, 1979                    +
 0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0060 REM
 0070 ESC
 0080 ON ESC THEN GOTO 1640
 0090 DIM D3$[10],F$[30],G$[8],H$[2],Q$[13],Q5$[132],Q6$[60],Q7$[30],Q8
*     $[133]
 0100 DIM Q9$[2],T$[6],U$[30],V$[8],V0$[20],V1$[40],V2$[11],V3$[40],V4$
*     [11],V5$[40],V6$[11],X$[3]
 0110 PAGE =132
 0120 LET Q6$="      ######################################  ########
*     ###"
 0130 REM   ----------------------------------------------------------------
 0140 REM          DETERMINE TYPE OF PROCESSING
 0150 READ FILE[4,1],T$,U$,N1,N2
 0160 ON N1 THEN GOTO 0170, 0190, 0210, 0230
 0170 LET Q7$="INTERNAL STANDARDS"
 0180 GOTO 0260
 0190 LET Q7$="PURGE AND TRAP"
 0200 GOTO 0260
 0210 LET Q7$="LIQUID/LIQUID EXTRACTION"
 0220 GOTO 0260
 0230 LET Q7$="DIRECT AQUEOUS INJECTION"
 0240 REM   ----------------------------------------------------------------
 0250 REM          SET EOF(3) AND EOF(4) BACK TO ZERO
 0260 CLOSE FILE[4]
 0270 OPEN FILE[4,0],T$,200
 0280 READ FILE[3,1],J,D3$
 0290 CLOSE FILE[3]
 0300 OPEN FILE[3,0],D3$,31
 0310 REM   ----------------------------------------------------------------
 0320 REM          COUNT IDENTIFIERS IN METHOD FILE
 0330 LET I5=0
 0340 READ FILE[4,3*(I5+1)-1],V$
 0350 IF EOF(4) THEN GOTO 0400
 0360 LET I5=I5+1
 0370 GOTO 0340
 0380 REM   ----------------------------------------------------------------

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                         PAGE  2
                        PROGRAM LISTING FOR GC13

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0390 REM          OPEN TEMPORARY FORMATTED OUTPUT FILE
 0400 LET Q$="GC0",T$[3,6]
 0410 OPEN FILE[5,1],Q$
 0420 REM   ----------------------------------------------------------------
 0430 REM          SKIP OVER ANY MESSAGES
 0440 LET P9=2
 0450 READ FILE[3,P9],V0$
 0460 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0510
 0470 LET P9=P9+1
 0480 GOTO 0450
 0490 REM   ----------------------------------------------------------------
 0500 REM          READ REPORT TITLE
 0510 LET P9=P9+1
 0520 READ FILE[3,P9],F$
 0530 REM   ----------------------------------------------------------------
 0540 REM          MATCH IDENTIFIER WITH NAME AND CAS NUMBFR
 0550 LET I6=1
 0560 READ FILF[3,I6+P9],G$,H$,B,C,L,L2
 0570 IF EOF(3) THEN GOTO 0960
 0580 IF G$="XXXXXXXX" THEN GOTO 0670
 0590 FOR I=1 TO I5
 0600   READ FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
 0610   IF V$=G$ THEN GOTO 0700
 0620 NEXT I
 0630 LET V1$="(",G$," - NOT IN METHOD ",T$[3,6],")"
 0640 LET V2$=""
 0650 LET V3$="99999"
 0660 GOTO 0700
 0670 LET V1$="    UNEXPLAINED PEAK"
 0680 LET V2$=""
 0690 LET V3$="99999"
 0700 LET Q5$="###.  ########################################  ########
*     ###   ##      ######                      "
 0702 IF C<>-9999 THEN GOTO 0710
 0704 LET Q5$=Q5$[1,60],"
*                 NOT DETECTED"
 0706 PRINT FILE[5],USING Q5$,I6,V1$,V2$
 0708 GOTO 0870
 0710 IF L2=-9999 THEN GOTO 0740
 0720 LET Q5$=Q5$,"  #####.##         "
 0730 GOTO 0750
 0740 LET Q5$=Q5$,"                   "

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                          PAGE  3
                        PROGRAM LISTING FOR GC13

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0750 LET Q5$=Q5$,"#########.#     "
 0760 IF L<>-9999 THEN GOTO 0765
 0762 IF G$<>"XXXXXXXX" THEN LET Q5$=Q5$," NOT CALCULATED"
 0763 GOTO 0770
 0765 LET Q5$=Q5$,"  -----#.###"
 0770 IF L=-9999 THEN IF L2=-9999 THEN GOTO 0820
 0780 IF L=-9999 THEN GOTO 0840
 0790 IF L2=-9999 THEN GOTO 0860
 0800 PRINT FILE[5],USING Q5$,I6,V1$,V2$,H$,B,L2,C,L
 0810 GOTO 0870
 0820 PRINT FILE[5],USING Q5$,I6,V1$,V2$,H$,B,C
 0830 GOTO 0870
 0840 PRINT FILE[5],USING Q5$,I6,V1$,V2$,H$,B,L2,C
 0850 GOTO 0870
 0860 PRINT FILE[5],USING Q5$,I6,V1$,V2$,H$,B,C,L
 0870 IF V3$="99999" THEN GOTO 0910
 0880 PRINT FILE[5],USING Q6$,V3$,V4$
 0890 IF V5$="99999" THEN GOTO 0910
 0900 PRINT FILE[5],USING Q6$,V5$,V6$
 0910 PRINT FILE[5]," "
 0920 LET I6=I6+1
 0930 GOTO 0560
 0940 REM  ------------------------------------------------------------
 0950 REM            PRINT HEADINGS ON LINEPRINTER
 0960 ON ERR THEN GOTO 0962
 0961 CLOSE FILE[3]
 0962 ON ERR THEN GOTO 0964
 0963 CLOSE FILE[5]
 0964 ON ERR THEN GOTO 0966
 0965 CLOSE FILE[6]
 0966 ON ERR THEN STOP
 0970 OPEN FILE[5,3],Q$
 0980 ON ERR THEN GOTO 1020
 0990 OPEN FILE[6,1],"$LPT"
 1000 ON ERR THEN STOP
 1010 GOTO 1050
 1020 ON ERR THEN STOP
 1030 DELAY =3
 1040 GOTO 0980
 1050 LET I7=1
 1060 PRINT FILE[6], TAB(49);"GAS CHROMATOGRAPHY AUTOMATION SYSTEM"
 1070 PRINT FILE[6]

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                          PAGE  4
                        PROGRAM LISTING FOR GC13

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 1080 PRINT FILE[6], TAB(34);"I-N-J-E-C-T-I-O-N   D-A-T-A   P-R-O-C-E-S
*     -S-I-N-G   R-E-P-O-R-T"
 1090 PRINT FILE[6]
 1100 PRINT FILE[6], TAB(29);
 1110 PRINT FILE[6],USING "ANALYST:  ##############################   I
*     NJECTION ID NUMBER:  ########",U$,D3$[3]
 1120 PRINT FILE[6], TAB(29);
 1130 PRINT FILE[6],USING "METHOD NUMBER:  ####                        R
*     EPORT TITLE:  ##############################",T$[3,6],F$
 1140 PRINT FILE[6], TAB(29);
 1150 PRINT FILE[6],USING "METHOD TYPE:  ############################# D
*     ATE:  ##/##/##",Q7$,SYS(2),SYS(1),SYS(3)-1900
 1160 PRINT FILE[6]
 1165 PRINT FILE[6]
 1170 GOSUB 1730
 1180 LET I6=12
 1190 REM  ------------------------------------------------------------
 1200 REM           COPY LINES FROM TEMPORARY FILE TO LINEPRINTER
 1210 LREAD FILE[5],Q8$,Q9$
 1220 IF EOF(5) THEN GOTO 1370
 1230 LET Q8$=Q8$,Q9$
 1240 PRINT FILE[6],Q8$
 1250 LET I6=I6+1
 1260 IF I6>58 THEN IF LEN(Q8$)<5 THEN GOTO 1280
 1270 GOTO 1210
 1280 LET I7=I7+1
 1281 LREAD FILE[5],Q8$,Q9$
 1282 IF EOF(5) THEN GOTO 1370
 1290 PRINT FILE[6],"<12>";
 1295 PRINT FILE[6], TAB(126);
 1300 PRINT FILE[6],USING "PAGE #",I7
 1310 PRINT FILE[6]
 1320 GOSUB 1730
 1330 LET I6=5
 1340 GOTO 1230
 1350 REM  ------------------------------------------------------------
 1360 REM           CONFIRM PROCESSING COMPLETION
 1370 PRINT
 1380 PRINT "INJECTION ";D3$[3];" HAS BEEN PROCESSED, AND A REPORT IS B
*     EING"
 1390 PRINT "    PRINTED BY THE LINEPRINTER."
 1400 ON ERR THEN GOTO 1402

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  5
                        PROGRAM LISTING FOR GC13

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 1401 CLOSE FILE[3]
 1402 ON ERR THEN GOTO 1404
 1403 CLOSE FILE[5]
 1404 ON ERR THEN GOTO 1410
 1405 CLOSE FILE[6]
 1410 ON ERR THEN GOTO 1430
 1420 DELETE Q$
 1430 ON ERR THEN STOP
 1440 PRINT
 1445 ON ERR THEN GOTO 1455
 1450 INPUT "DO YOU WANT TO PROCESS ANOTHER INJECTION USING THE SAME ME
*     THOD?  (Y OR N)  ",X$
 1455 ON ERR THEN STOP
 1460 IF X$[1,1]<>"Y" THEN GOTO 1680
 1540 REM   ----------------------------------------------------------
 1550 REM           PROCESS ANOTHER INJECTION
 1560 NOESC
 1570 ON N1 THEN GOTO 1580, 1590, 1600, 1610
 1580 CHAIN "GC08"
 1590 CHAIN "GC09"
 1600 CHAIN "GC10"
 1610 CHAIN "GC11"
 1620 REM   ----------------------------------------------------------
 1630 REM           RETURN TO MASTER CONTROL
 1640 ON ERR THEN GOTO 1642
 1641 CLOSE FILE[3]
 1642 ON ERR THEN GOTO 1644
 1643 CLOSE FILE[5]
 1644 ON ERR THEN GOTO 1650
 1645 CLOSE FILE[6]
 1650 ON ERR THEN GOTO 1670
 1660 DELETE Q$
 1670 ON ESC THEN STOP
 1680 NOESC
 1690 CHAIN "GC00"
 1700 REM
 1710 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 1720 REM           SUBROUTINE TO PRINT COLUMN HEADINGS
 1730 PRINT FILE[6], TAB(51);"C.A.S.    PEAK     RETENTION    ";
 1740 IF N2<>1 THEN GOTO 1770
 1750 PRINT FILE[6],"   RELATIVE     ";
 1760 GOTO 1780

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  6
                        PROGRAM LISTING FOR GC13

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 1770 PRINT FILE[6],"   CAPACITY     ";
 1780 PRINT FILE[6],"    AREA OF      CONCENTRATION IN"
 1790 PRINT FILE[6], TAB(21);"COMPOUND(S)                    NUMBER    T
*     YPE       TIME        ";
 1800 IF N2<>1 THEN GOTO 1830
 1810 PRINT FILE[6],"RETENTION TIME  ";
 1820 GOTO 1840
 1830 PRINT FILE[6],"    RATIO        ";
 1840 PRINT FILE[6],"     PEAK        MICROGRAMS/LITER"
 1850 PRINT FILE[6],"      ----------------------------------------  --
*     ---------  ----";
 1860 PRINT FILE[6]," --------------  --------------  --------------
*     ----------------"
 1870 RETURN

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  7
                        SYMBOL TABLE FOR GC13

SYMBOL   REFERENCES
-------  ------------------------------------------------------------
 0170    0160
 0190    0160
 0210    0160
 0230    0160
 0260    0180  0200  0220
 0340    0370
 0400    0350
 0450    0480
 0510    0460
 0560    0930
 0670    0580
 0700    0610  0660
 0710    0702
 0740    0710
 0750    0730
 0765    0760
 0770    0763
 0820    0770
 0840    0780
 0860    0790
 0870    0708  0810  0830  0850
 0910    0870  0890
 0960    0570
 0962    0960
 0964    0962
 0966    0964
 0980    1040
 1020    0980
 1050    1010
 1210    1270
 1230    1340
 1280    1260
 1370    1220  1282
 1402    1400
 1404    1402
 1410    1404
 1420    1410
 1455    1445
 1580    1570
 1590    1570
 1600    1570
 1610    1570
 1640    0080
 1642    1640
 1644    1642
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  8
                        SYMBOL TABLE FOR GC13

SYMBOL   REFERENCES
-------  ------------------------------------------------------------
 1650    1644
 1670    1650
 1680    1460
 1730    1170  1320
 1770    1740
 1780    1760
 1830    1800
 1840    1820
 B       0560  0800  0820  0840  0860
 C       0560  0702  0800  0820  0840  0860
 D3$     0090  0280  0300  1110  1380
 F$      0090  0520  1130
 FL#3    0280  0290  0300  0450  0520  0560  0961  1401  1641
 FL#4    0150  0260  0270  0340  0600
 FL#5    0410  0706  0800  0820  0840  0860  0880  0900  0910  0963
         0970  1210  1281  1403  1643
 FL#6    0965  0990  1060  1070  1080  1090  1100  1110  1120  1130
         1140  1150  1160  1165  1240  1290  1295  1300  1310  1405
         1645  1730  1750  1770  1780  1790  1810  1830  1840  1850
         1860
 G$      0090  0560  0580  0610  0630  0762
 H$      0090  0560  0800  0820  0840  0860
 I       0590  0600  0620
 I5      0330  0340  0360  0590
 I6      0550  0560  0706  0800  0820  0840  0860  0920  1180  1250
         1260  1330
 I7      1050  1280  1300
 J       0280
 L       0560  0760  0770  0780  0800  0860
 L2      0560  0710  0770  0790  0800  0840
 N1      0150  0160  1570
 N2      0150  1740  1800
 P9      0440  0450  0470  0510  0520  0560
 Q$      0090  0400  0410  0970  1420  1660
 Q5$     0090  0700  0704  0706  0720  0740  0750  0762  0765  0800
         0820  0840  0860
 Q6$     0090  0120  0880  0900
 Q7$     0090  0170  0190  0210  0230  1150
 Q8$     0090  1210  1230  1240  1260  1281
 Q9$     0100  1210  1230  1281
 T$      0100  0150  0270  0400  0630  1130
 U$      0100  0150  1110
 V$      0100  0340  0600  0610
 V0$     0100  0450  0460
 V1$     0100  0600  0630  0670  0706  0800  0820  0840  0860
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  9
                         SYMBOL TABLE FOR GC13

SYMBOL   REFERENCES
------   ------------------------------------------------------------
 V2$     0100  0600  0640  0680  0706  0800  0820  0840  0860
 V3$     0100  0600  0650  0690  0870  0880
 V4$     0100  0600  0880
 V5$     0100  0600  0890  0900
 V6$     0100  0600  0900
 X$      0100  1450  1460
```

SECTION 16

PROGRAM GC14 - CONTROL STANDARDS CALCULATION

GC14 is the program which calculates percent recoveries for control standards and prints the control standard report. It is entered by chaining from the master control program, GC00, and it returns control to that program if the escape key is pressed.

As GC14 begins, a method file is already open, having been opened by GC00. GC14 first counts the identifiers in the method file. It then asks the user for the injection ID of the control standard and opens the corresponding injection data file. It also asks the user for the letter name of the concentration pattern and opens the concentration pattern file.

Next, GC14 prints the headings for the control standard report. It then loops through the method file. For each identifier in the method file, GC14 reads the prepared concentration from the concentration pattern file and searches the data file for the calculated concentration. It then prints the identifier, the prepared concentration, the calculated concentration, and the percent recovery on the control standard report. Percent recovery is calculated by the formula:

$$\text{Percent Recovery} = 100 \bullet \frac{\text{Measured Concentration}}{\text{Prepared Concentration}}$$

When all of the identifiers have been covered, the program closes the concentration pattern file and the data file, and it asks if the user wants to examine another control standard. It then either branches back to the beginning or chains back to GC00.

TABLE 10. SYMBOL DEFINITIONS FOR PROGRAM GC14

A5	the prepared concentration
A6$	the name of the concentration pattern file
A7	the position of A8$ in A9$
A8$	the letter name of the concentration pattern
A9$	the alphabet
B	the absolute retention time
C	the peak area
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I2	the control variable for a loop
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 has been processed J2=2 never processed
L	the calculated concentration
L2	the relative retention time or capacity ratio

TABLE 10. (Continued)

P8	the record number of the last record in the data file
P9	the record number of the first record in the data file which represents a peak
Q5$	the format for a PRINT USING statement
T$	the name of the method file
V$	an identifier from the method file
VO$	an error message
X$	the user's answer to Y or N questions

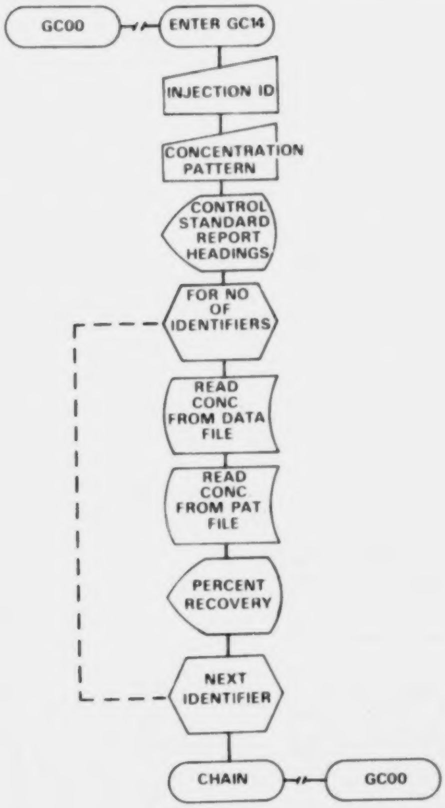

GC00
ENTER GC14
INJECTION ID
CONCENTRATION PATTERN
CONTROL STANDARD REPORT HEADINGS
FOR NO OF IDENTIFIERS
READ CONC FROM DATA FILE
READ CONC FROM PAT FILE
PERCENT RECOVERY
NEXT IDENTIFIER
CHAIN
GC00

Figure 12. Flowchart of Program GC14.

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                       PROGRAM LISTING FOR GC14

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                   +
0030 REM   +   PROGRAM GC14, CONTROL STANDARDS CALCULATIONS           +
0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 3, 1979                  +
0050 REM   +   MOST RECENT REVISION:  APRIL 12, 1979                  +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM A6$[9],A8$[1],A9$[26],D2$[8],D3$[10],G$[8],H$[2],Q5$[80],T$[6
*    ],V$[8],V0$[30],X$[3]
0090 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
0100 ON ESC THEN GOTO 0130
0110 ESC
0120 GOTO 0220
0130 ON ERR THEN GOTO 0150
0140 CLOSE FILE[3]
0150 ON ERR THEN GOTO 0170
0160 CLOSE FILE[7]
0170 ON ERR THEN STOP
0180 NOESC
0190 CHAIN "GC00"
0200 REM  -------------------------------------------------------------
0210 REM            COUNT IDENTIFIERS IN METHOD FILE
0220 READ FILE[4,1],T$
0230 CLOSE FILE[4]
0240 OPEN FILE[4],T$,200
0250 LET F=0
0260 READ FILE[4,3*(F+1)-1],V$
0270 IF EOF(4) THEN GOTO 032C
0280 LET F=F+1
0290 GOTO 0260
0300 REM  -------------------------------------------------------------
0310 REM            OPEN DATA FILE
0320 PRINT
0330 ON ERR THEN GOTO 0350
0340 INPUT "WHAT IS THE INJECTION ID FOR THE CONTROL STANDARD?  ",D2$
0350 ON ERR THEN STOP
0360 IF LEN(D2$)=8 THEN GOTO 0400
0370 PRINT
0380 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0390 GOTO 0320
0400 LET D3$="GC",D2$
0410 ON ERR THEN GOTO 0430

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                       PROGRAM LISTING FOR GC14

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0420 RENAME D3$,D3$
0430 ON ERR THEN STOP
0440 IF SYS(7)=-9 THEN GOTO 0480
0450 PRINT
0460 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0470 GOTO 0320
0480 ON ERR THEN GOTO 0520
0490 OPEN FILE[3,0],D3$,31
0500 ON ERR THEN STOP
0510 GOTO 0570
0520 ON ERR THEN STOP
0530 DELAY =1
0540 GOTO 0480
0550 REM  -------------------------------------------------------------
0560 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
0570 READ FILE[3,1],J,D3$,J2
0580 IF J=1 THEN GOTO 0630
0590 PRINT
0600 IF J<>2 THEN GOTO 0610
0602 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
0604 PRINT "     HAVE A TOTAL AREA"
0606 GOTO 1420
0610 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
0612 PRINT "     IN THE WRONG FORMAT."
0620 GOTO 1420
0630 IF J2=1 THEN GOTO 0690
0640 PRINT
0650 PRINT "<7><7>";D2$;" CANNOT BE USED FOR CONTROL STANDARD CALCULAT
*    IONS UNTIL"
0652 PRINT "     AFTER IT IS PROCESSED."
0660 GOTO 0130
0670 REM  -------------------------------------------------------------
0680 REM          FIND FIRST AND LAST ENTRIES IN DATA FILE
0690 LET P9=2
0700 READ FILE[3,P9],V0$
0710 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0740
0720 LET P9=P9+1
0730 GOTO 0700
0740 LET P9=P9+2
0750 LET P8=P9
0760 READ FILE[3,P8],G$
0770 IF EOF(3) THEN GOTO 0800

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                        PAGE  3
                         PROGRAM LISTING FOR GC14

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0780 LET P8=P8+1
 0790 GOTO 0760
 0800 LET P8=P8-1
 0810 REM   -----------------------------------------------------------
 0820 REM           OPEN CONCENTRATION PATTERN FILE
 0830 PRINT
 0840 ON ERR THEN GOTO 0860
 0850 INPUT "WHAT IS THE CONCENTRATION PATTERN FOR THIS STANDARD?  ",A8
*     $
 0860 ON ERR THEN STOP
 0R70 LET A7=POS(A9$,A8$,1)
 0880 IF A7<>0 THEN GOTO 0920
 0890 PRINT
 0900 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
 0910 GOTO 0830
 0920 LET A6$=T$,"000"
 0930 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
 0940 ON ERR THEN GOTO 0960
 0950 RENAME A6$,A6$
 0960 ON ERR THEN STOP
 0970 IF SYS(7)=-9 THEN GOTO 1010
 0980 PRINT
 0990 PRINT "<7><7>THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
 1000 GOTO 0830
 1010 ON ERR THEN GOTO 1050
 1020 OPEN FILE[7,0],A6$,4
 1030 ON ERR THEN STOP
 1040 GOTO 1100
 1050 ON ERR THEN STOP
 1060 DELAY =1
 1070 GOTO 1010
 1080 REM   -----------------------------------------------------------
 1090 REM           PRINT HEADINGS
 1100 PRINT
 1110 PRINT
 1120 PRINT  TAB(15);"C-O-N-T-R-O-L   S-T-A-N-D-A-R-D   R-E-P-O-R-T"
 1130 PRINT "INJECTION ID:  ";D2$; TAB(53);"METHOD NUMBER:  ";T$[3,6]
 1140 PRINT "CONCENTRATION PATTERN:  ";A8$; TAB(39);"CONCENTRATIONS IN
*     MICROGRAMS/LITER"
 1150 PRINT
 1160 PRINT "              PREPARED        MEASURED       PERCENT"
 1170 PRINT "IDENTIFIER  CONCENTRATION  CONCENTRATION  RECOVERED"

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                        PAGE  4
                         PROGRAM LISTING FOR GC14

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 1180 PRINT "----------  ------------  ------------  ---------"
 1190 LET Q5$=" ########    -----#.###     -----#.###      ---#.#%"
 1195 REM   -----------------------------------------------------------
 1196 REM           FILL IN TABLE
 1200 FOR I=1 TO F
 1210   READ FILE[4,3*I-1],V$
 1215   IF V$="99999" THEN GOTO 1360
 1220   READ FILE[7,I],A5
 1230   FOR I2=P9 TO P8 STEP 1
 1240     READ FILE[3,I2],G$,H$,B,C,L,L2
 1250     IF G$=V$ THEN GOTO 1270
 1260   NEXT I2
 1265   LET C=-9999
 1266   LET L=-9999
 1270   IF C<>-9999 THEN GOTO 1310
 1280   PRINT USING Q5$[1,27],V$,A5;
 1290   PRINT "NOT DETECTED"
 1300   GOTO 1360
 1310   IF L<>-9999 THEN GOTO 1350
 1320   PRINT USING Q5$[1,27],V$,A5;
 1330   PRINT "NOT CALCULATED"
 1340   GOTO 1360
 1350   PRINT USING Q5$,V$,A5,L,L/A5*100
 1360 NEXT I
 1370 PRINT
 1380 PRINT
 1390 REM   -----------------------------------------------------------
 1400 REM           WRAP-UP PROCEDURE
 1410 CLOSE FILE[7]
 1420 CLOSE FILE[3]
 1430 PRINT
 1440 ON ERR THEN GOTO 1460
 1450 INPUT "DO YOU WANT A REPORT ON ANOTHER CONTROL STANDARD?  (Y OR N
*     )  ",X$
 1460 ON ERR THEN STOP
 1470 IF X$[1,1]="Y" THEN GOTO 0320
 1480 NOESC
 1490 CHAIN "GC00"

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                  PAGE  5
                      SYMBOL TABLE FOR GC14

SYMBOL    REFERENCES
------  ----------------------------------------------------------
 0130   0100  0660
 0150   0130
 0170   0150
 0220   0120
 0260   0290
 0320   0270  0390  0470  1470
 0350   0330
 0400   0360
 0430   0410
 0480   0440  0540
 0520   0480
 0570   0510
 0610   0600
 0630   0580
 0690   0630
 0700   0730
 0740   0710
 0760   0790
 0800   0770
 0830   0910  1000
 0860   0840
 0920   0880
 0960   0940
 1010   0970  1070
 1050   1010
 1100   1040
 1270   1250
 1310   1270
 1350   1310
 1360   1215  1300  1340
 1420   0606  0620
 1460   1440
 A5     1220  1280  1320  1350
 A6$    0080  0920  0930  0950  1020
 A7     0870  0880  0930
 A8$    0080  0850  0870  0900  0990  1140
 A9$    0080  0090  0870
 B      1240
 C      1240  1265  1270
 D2$    0080  0340  0360  0380  0400  0460  0602  0610  0650  1130
 D3$    0080  0400  0420  0490  0570
 F      0250  0260  0280  1200
 Fl.#3  0140  0490  0570  0700  0760  1240  1420
 FL#4   0220  0230  0240  0260  1210
 FL#7   0160  1020  1220  1410
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                  PAGE  6
                      SYMBOL TABLE FOR GC14

SYMBOL    REFERENCES
------  ----------------------------------------------------------
 G$     0080  0760  1240  1250
 H$     0080  1240
 I      1200  1210  1220  1360
 I2     1230  1240  1260
 J      0570  0580  0600
 J2     0570  0630
 L      1240  1266  1310  1350
 L2     1240
 P8     0750  0760  0780  0800  1230
 P9     0690  0700  0720  0740  0750  1230
 Q5$    0080  1190  1280  1320  1350
 T$     0080  0220  0240  0920  1130
 V$     0080  0260  1210  1215  1250  1280  1320  1350
 VO$    0080  0700  0710
 X$     0080  1450  1470
```

SECTION 17

PROGRAM GC15 - SPIKED SAMPLES CALCULATION

GC15 is the program which calculates the percent recovery of spiked samples and prints a report on those statistics. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

As GC15 begins, a method file is already open, having been opened by GC00. GC15 first counts the identifiers in the method file. Then it asks the user for the injection ID of the spike original, the letter name of the concentration pattern for the spike added value, and the injection ID of the spike final, and it opens the three corresponding files.

Next, the program prints the headings for the spiked sample report. It then loops through the method file. It reads an identifier from the method file and reads the spike added value from the concentration pattern file. It loops through the first injection data file, finds the matching identifier and reads its calculated concentration, and then loops through the second injection data file, finds the matching identifier there, and reads its calculated concentration. The percent recovery is calculated as the line of data is printed. Percent recovery of spikes is calculated by the formula:

$$\text{Percent Recovery} = \frac{\text{Final Concentration} - \text{Original Concentration}}{\text{Added Concentration}}$$

When all of the identifiers in the method file have been handled, the program either starts over or chains back to GC00, at the option of the user.

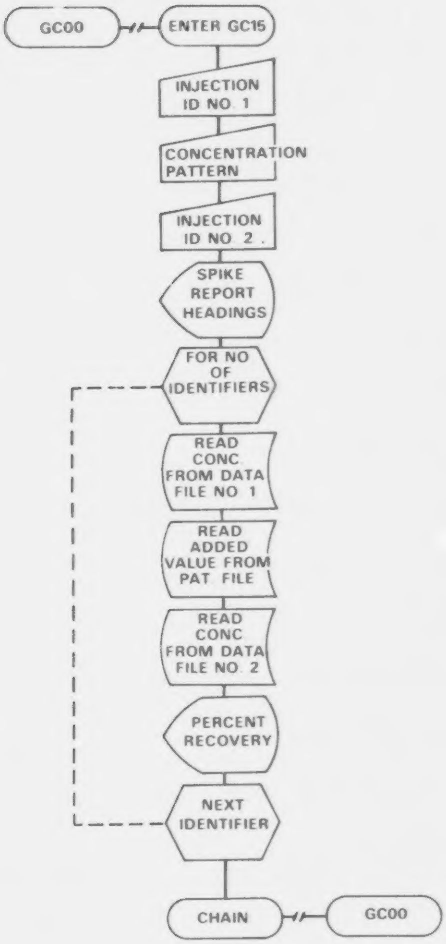

GC00
ENTER GC15
INJECTION ID NO. 1
CONCENTRATION PATTERN
INJECTION ID NO. 2 .
SPIKE REPORT HEADINGS
FOR NO OF IDENTIFIERS
READ CONC. FROM DATA FILE NO. 1
READ ADDED VALUE FROM PAT. FILE
READ CONC FROM DATA FILE NO. 2
PERCENT RECOVERY
NEXT IDENTIFIER
CHAIN
GC00

Figure 13. Flowchart of Program GC15.

TABLE 11. SYMBOL DEFINITIONS FOR PROGRAM GC15

A5	the spike added concentration
A6$	the name of the concentration pattern file
A7	the position of A8$ in A9$
A8$	the letter name of the concentration pattern
A9$	the alphabet
B	the absolute retention time
C	the peak area of the spike original
C2	the peak area of the spike final
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I2	the control variable for loops
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 has been processed J2=2 never processed
L	the relative retention time

TABLE 11. (Continued)

L2	the calculated concentration of the spike original
L3	the calculated concentration of the spike final
P6	the record number of the last record in the spike final data file
P7	the record number of the first record which describes a peak in the spike final data file
P8	the record number of the last record in the spike original data file
P9	the record number of the first record which describes a peak in the spike original data file
T$	the name of the method file
V$	the identifier from the method file
VO$	an error MESSAGE
X$	the user's response to Y or N questions

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE  1
                     PROGRAM LISTING FOR GC15

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM  +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM  +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM  +   PROGRAM GC15, SPIKED SAMPLE CALCULATIONS                +
0040 REM  +   BY:  J. KOPKE (SWORCC), APRIL 5, 1979                   +
0050 REM  +   MOST RECENT REVISION:  MAY 2, 1979                      +
0060 REM  +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM A6$[9],A8$[1],A9$[26],D2$[8],D3$[10],G$[8],H$[2],T$[6],V$[8],
*     V0$[30],X$[3]
0090 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
0100 ON ESC THEN GOTO 0130
0110 ESC
0120 GOTO 0240
0130 ON ERR THEN GOTO 0150
0140 CLOSE FILE[3]
0150 ON ERR THEN GOTO 0170
0160 CLOSE FILE[7]
0170 ON ERR THEN GOTO 0190
0180 CLOSE FILE[0]
0190 ON ERR THEN STOP
0200 NOESC
0210 CHAIN "GC00"
0220 REM  ------------------------------------------------------------
0230 REM           COUNT IDENTIFIERS IN METHOD FILE
0240 READ FILE[4,1],T$
0250 CLOSE FILE[4]
0260 OPEN FILE[4],T$,200
0270 LET F=0
0280 READ FILE[4,3*(F+1)-1],V$
0290 IF EOF(4) THEN GOTO 0340
0300 LET F=F+1
0310 GOTO 0280
0320 REM  ------------------------------------------------------------
0330 REM           OPEN SPIKE ORIGINAL DATA FILE
0340 PRINT
0350 ON ERR THEN GOTO 0370
0360 INPUT "WHAT IS THE INJECTION ID FOR THE UNSPIKED SAMPLE?  ",D2$
0370 ON ERR THEN STOP
0380 IF LEN(D2$)=8 THEN GOTO 0420
0390 PRINT
0400 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0410 GOTO 0340

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE  2
                     PROGRAM LISTING FOR GC15

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0420 LET D3$="GC",D2$
0430 ON ERR THEN GOTO 0450
0440 RENAME D3$,D3$
0450 ON ERR THEN STOP
0460 IF SYS(7)=-9 THEN GOTO 0500
0470 PRINT
0480 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0490 GOTO 0340
0500 ON ERR THEN GOTO 0540
0510 OPEN FILE[3,0],D3$,31
0520 ON ERR THEN STOP
0530 GOTO 0590
0540 ON ERR THEN STOP
0550 DELAY =1
0560 GOTO 0500
0570 REM  ------------------------------------------------------------
0580 REM           CHECK DATA FILE USABILITY AND PROCESSING FLAGS
0590 READ FILE[3,1],J,D3$,J2
0600 IF J=1 THEN GOTO 0690
0610 PRINT
0620 IF J<>2 THEN GOTO 0660
0630 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
0640 PRINT "     HAVE A TOTAL AREA"
0650 GOTO 2250
0660 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
0670 PRINT "     IN THE WRONG FORMAT."
0680 GOTO 2250
0690 IF J2=1 THEN GOTO 0760
0700 PRINT
0710 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SPIKED SAMPLE CALCULATION
*     S UNTIL"
0720 PRINT "     AFTER IT IS PROCESSED."
0730 GOTO 0130
0740 REM  ------------------------------------------------------------
0750 REM           FIND FIRST AND LAST ENTRIES IN DATA FILE
0760 LET P9=2
0770 READ FILE[3,P9],V0$
0780 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0810
0790 LET P9=P9+1
0800 GOTO 0770
0810 LET P9=P9+2
0820 LET P8=P9

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                        PAGE  3
                     PROGRAM LISTING FOR GC15

1234567891123456789212345678931234567894123456789512345678961234567897
         0          0          0          0          0          0          0
0830 READ FILE[3,P8],G$
0840 IF EOF(3) THEN GOTO 0870
0850 LET P8=P8+1
0860 GOTO 0830
0870 LET P8=P8-1
0880 REM  ------------------------------------------------------------
0890 REM           OPEN CONCENTRATION PATTERN FILE
0900 PRINT
0910 ON ERR THEN GOTO 0930
0920 INPUT "WHAT IS THE CONCENTRATION PATTERN FOR THE SPIKE ADDED VALU
*     ES?  ",A8$
0930 ON ERR THEN STOP
0940 LET A7=POS(A9$,A8$,1)
0950 IF A7<>0 THEN GOTO 0990
0960 PRINT
0970 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
0980 GOTO 0900
0990 LET A6$=T$,"000"
1000 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
1010 ON ERR THEN GOTO 1030
1020 RENAME A6$,A6$
1030 ON ERR THEN STOP
1040 IF SYS(7)=-9 THEN GOTO 1080
1050 PRINT
1060 PRINT "<7><7>THERF IS NO EXISTING PATTERN NAMED '";A8$;"'."
1070 GOTO 0900
1080 ON ERR THEN GOTO 1120
1090 OPEN FILE[7,0],A6$,4
1100 ON ERR THEN STOP
1110 GOTO 1170
1120 ON ERR THEN STOP
1130 DELAY =1
1140 GOTO 1080
1150 REM  ------------------------------------------------------------
1160 REM           OPEN SPIKE FINAL DATA FILE
1170 PRINT
1180 ON ERR THEN GOTO 1200
1190 INPUT "WHAT IS THE INJECTION ID FOR THE SPIKED SAMPLE?  ",D2$
1200 ON ERR THEN STOP
1210 IF LEN(D2$)=8 THEN GOTO 1250
1220 PRINT
1230 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."

1234567891123456789212345678931234567894123456789512345678961234567897
         0          0          0          0          0          0          0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/24/1979                                                        PAGE  4
                     PROGRAM LISTING FOR GC15

1234567891123456789212345678931234567894123456789512345678961234567897
         0          0          0          0          0          0          0
1240 GOTO 1170
1250 LET D3$="GC",D2$
1260 ON ERR THEN GOTO 1280
1270 RENAME D3$,D3$
1280 ON ERR THEN STOP
1290 IF SYS(7)=-9 THEN GOTO 1330
1300 PRINT
1310 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
1320 GOTO 1170
1330 ON ERR THEN GOTO 1370
1340 OPEN FILE[0,0],D3$,31
1350 ON ERR THEN STOP
1360 GOTO 1420
1370 ON ERR THEN STOP
1380 DELAY =1
1390 GOTO 1330
1400 REM  ------------------------------------------------------------
1410 REM           CHECK DATA FILE USABILITY AND PROCESSING FLAGS
1420 READ FILE[0,1],J,D3$,J2
1430 IF J=1 THEN GOTO 1520
1440 PRINT
1450 IF J<>2 THEN GOTO 1490
1460 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
1470 PRINT "     HAVE A TOTAL AREA"
1480 GOTO 2250
1490 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
1500 PRINT "     IN THE WRONG FORMAT."
1510 GOTO 2250
1520 IF J2=1 THEN GOTO 1590
1530 PRINT
1540 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SPIKED SAMPLE CALCULATION
*     S UNTIL"
1550 PRINT "     AFTER IT IS PROCESSED."
1560 GOTO 0130
1570 REM  ------------------------------------------------------------
1580 REM           FIND FIRST AND LAST ENTRIES IN DATA FILE
1590 LET P7=2
1600 READ FILE[0,P7],V0$
1610 IF V0$[1,7]<>"MESSAGE" THEN GOTO 1640
1620 LET P7=P7+1
1630 GOTO 1600
1640 LET P7=P7+2

1234567891123456789212345678931234567894123456789512345678961234567897
         0          0          0          0          0          0          0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  5
                          PROGRAM LISTING FOR GC15

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1650 LET P6=P7
1660 READ FILE[0,P6],G$
1670 IF EOF(0) THEN GOTO 1700
1680 LET P6=P6+1
1690 GOTO 1660
1700 LET P6=P6-1
1710 REM   ------------------------------------------------------------
1720 REM          PRINT HEADINGS
1730 PRINT
1740 PRINT
1750 PRINT  TAB(17);"S-P-I-K-E-D  S-A-M-P-L-E  R-E-P-O-R-T"
1760 READ FILE[3,1],J,D3$,J2
1770 PRINT "INJECTION ID FOR SPIKE ORIGINAL:  ";D3$[3,10]; TAB(53);"ME
*    THOD NUMBER:  ";T$[3,6]
1780 PRINT "CONCENTRATION PATTERN FOR SPIKE ADDED VALUE:  ";A8$
1790 READ FILE[0,1],J,D3$,J2
1800 PRINT "INJECTION ID FOR SPIKE FINAL:  ";D3$[3,10]
1810 PRINT "CONCENTRATIONS IN MICROGRAMS/LITER"
1820 PRINT
1830 PRINT "              ORIGINAL        ADDED          FINAL
*    PERCENT"
1840 PRINT "IDENTIFIER  CONCENTRATION  CONCENTRATION  CONCENTRATION  R
*    ECOVERED"
1850 PRINT "----------  -------------  -------------  -------------  -
*    --------"
1860 REM   ------------------------------------------------------------
1870 REM          FILL IN CHART
1880 FOR I=1 TO F
1890   READ FILE[4,3*I-1],V$
1900   IF V$="99999" THEN GOTO 2200
1910   READ FILE[7,I],A5
1920   FOR I2=P9 TO P8
1930     READ FILE[3,I2],G$,H$,B,C,L,L2
1940     IF G$=V$ THEN GOTO 1960
1950   NEXT I2
1955   LET C=-9999
1956   LET L=-9999
1960   FOR I2=P7 TO P6
1970     READ FILE[0,I2],G$,H$,B,C2,L3,L2
1980     IF G$=V$ THEN GOTO 2000
1990   NEXT I2
1995   LET C2=-9999

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  6
                          PROGRAM LISTING FOR GC15

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1996   LET L3=-9999
2000   PRINT USING " ########   ",V$;
2010   IF C<>-9999 THEN GOTO 2040
2020   PRINT " NOT DETECTED  ";
2030   GOTO 2080
2040   IF L<>-9999 THEN GOTO 2070
2050   PRINT "NOT CALCULATED ";
2060   GOTO 2080
2070   PRINT USING "-----#.###     ",L;
2080   PRINT USING "-----#.###     ",A5;
2090   IF C2<>-9999 THEN GOTO 2120
2100   PRINT " NOT DETECTED  ";
2110   GOTO 2160
2120   IF L3<>-9999 THEN GOTO 2150
2130   PRINT "NOT CALCULATED ";
2140   GOTO 2160
2150   PRINT USING "-----#.###     ",L3;
2160   IF C<>-9999 THEN IF L<>-9999 THEN IF C2<>-9999 THEN IF L3<>-999
*    9 THEN GOTO 2190
2170   PRINT
2180   GOTO 2200
2190   PRINT USING "---#.#%",(L3-L)/A5*100
2200 NEXT I
2210 PRINT
2220 PRINT
2230 REM   ------------------------------------------------------------
2240 REM          WRAP-UP PROCEDURE
2250 ON ERR THEN GOTO 2270
2260 CLOSE FILE[0]
2270 ON ERR THEN GOTO 2290
2280 CLOSE FILE[3]
2290 ON ERR THEN GOTO 2310
2300 CLOSE FILE[7]
2310 ON ERR THEN STOP
2320 PRINT
2330 ON ERR THEN GOTO 2350
2340 INPUT "DO YOU WANT A REPORT FOR ANOTHER SPIKED SAMPLE?  (Y OR N)
*    ",X$
2350 ON ERR THEN STOP
2360 IF X$[1,1]="Y" THEN GOTO 0340
2370 NOESC
2380 CHAIN "GC00"

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                        PAGE  7
                         SYMBOL TABLE FOR GC15

SYMBOL   REFERENCES
------  --------------------------------------------------------------
 0130  0100  0730  1560
 0150  0130
 0170  0150
 0190  0170
 0240  0120
 0280  0310
 0340  0290  0410  0490  2360
 0370  0350
 0420  0380
 0450  0430
 0500  0460  0560
 0540  0500
 0590  0530
 0660  0620
 0690  0600
 0760  0690
 0770  0800
 0810  0780
 0830  0860
 0870  0840
 0900  0980  1070
 0930  0910
 0990  0950
 1030  1010
 1080  1040  1140
 1120  1080
 1170  1110  1240  1320
 1200  1180
 1250  1210
 1280  1260
 1330  1290  1390
 1370  1330
 1420  1360
 1490  1450
 1520  1430
 1590  1520
 1600  1630
 1640  1610
 1660  1690
 1700  1670
 1960  1940
 2000  1980
 2040  2010
 2070  2040
 2080  2030  2060
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                        PAGE  8
                         SYMBOL TABLE FOR GC15

SYMBOL   REFERENCES
------  --------------------------------------------------------------
 2120  2090
 2150  2120
 2160  2110  2140
 2190  2160
 2200  1900  2180
 2250  0650  0680  1480  1510
 2270  2250
 2290  2270
 2310  2290
 2350  2330
 A5    1910  2080  2190
 A6$   0080  0990  1000  1020  1090
 A7    0940  0950  1000
 A8$   0080  0920  0940  0970  1060  1780
 A9$   0080  0090  0940
 B     1930  1970
 C     1930  1955  2010  2160
 C2    1970  1995  2090  2160
 D2$   0080  0360  0380  0400  0420  0480  0630  0660  0710  1190
       1210  1230  1250  1310  1460  1490  1540
 D3$   0080  0420  0440  0510  0590  1250  1270  1340  1420  1760
       1770  1790  1800
 F     0270  0280  0300  1880
 FL#0  0180  1340  1420  1600  1660  1790  1970  2260
 FL#3  0140  0510  0590  0770  0830  1760  1930  2280
 FL#4  0240  0250  0260  0280  1890
 FL#7  0160  1090  1910  2300
 G$    0080  0830  1660  1930  1940  1970  1980
 H$    0080  1930  1970
 I     1880  1890  1910  2200
 I2    1920  1930  1950  1960  1970  1990
 J     0590  0600  0620  1420  1430  1450  1760  1790
 J2    0590  0690  1420  1520  1760  1790
 L     1930  1956  2040  2070  2160  2190
 L2    1930  1970
 L3    1970  1996  2120  2150  2160  2190
 P6    1650  1660  1680  1700  1960
 P7    1590  1600  1620  1640  1650  1960
 P8    0820  0830  0850  0870  1920
 P9    0760  0770  0790  0810  0820  1920
 T$    0080  0240  0260  0990  1770
 V$    0080  0280  1890  1900  1940  1980  2000
 V0$   0080  0770  0780  1600  1610
 X$    0080  2340  2360
```

SECTION 18

PROGRAM GC16 - DUPLICATE SAMPLES CALCULATION

GC16 is the program which calculates the difference between duplicate samples and prints a report on those statistics. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

When GC16 begins, the method file is already open, and GC16 first counts the number of identifiers in that method file. Then the program asks the user for the injection ID numbers for the two members of the duplicate pair, and it opens the two corresponding injection data files.

After the headings have been printed, the program begins to loop through the method file. It reads an identifier from the method file and searches the two data files for that identifier. It reads the concentrations from the data files, and prints them and their absolute difference.

When all of the identifiers have been accounted for, the program asks the user if it should start over. It then either branches back to the beginning or chains back to GC00.

TABLE 12. SYMBOL DEFINITIONS FOR PROGRAM GC16

B	the absolute retention time
C	the peak area of the first member
C2	the peak area of the second member
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I2	the control variable for loops
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 has been processed J2=2 never processed
L	the relative retention time
L2	the calculated concentration of the first member
L3	the calculated concentration of the second member

TABLE 12. (Continued)

P6	the record number of the last record in the second member data file
P7	the record number of the first record which describes a peak in the second member data file
P8	the record number of the last record in the first member data file
P9	the record number of the first record which describes a peak in the first member data file
T$	the name of the method file
V$	the identifier from the method file
VO$	an error MESSAGE
X$	the user's response to Y or N questions

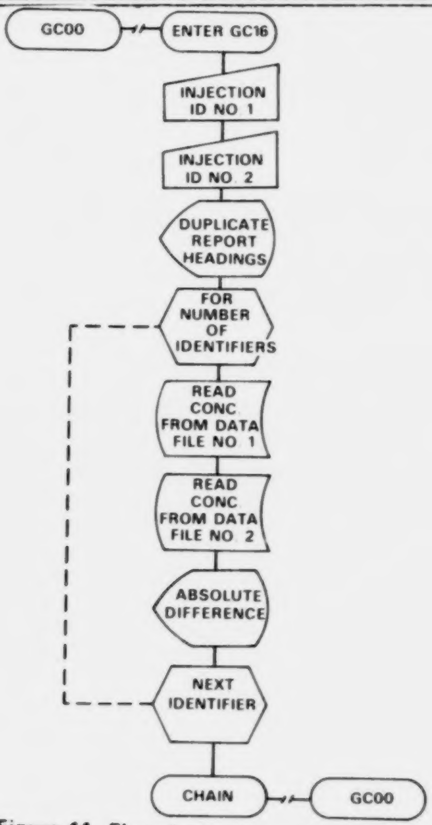

GC00
ENTER GC16
INJECTION ID NO 1
INJECTION ID NO 2
DUPLICATE REPORT HEADINGS
FOR NUMBER OF IDENTIFIERS
READ CONC FROM DATA FILE NO 1
READ CONC FROM DATA FILE NO 2
ABSOLUTE DIFFERENCE
NEXT IDENTIFIER
CHAIN
GC00

Figure 14. Flowchart of Program GC16.

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                     PROGRAM LISTING FOR GC16

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC16, DUPLICATE SAMPLES CALCULATIONS            +
0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 9, 1979                   +
0050 REM   +   MOST RECENT REVISION:  APRIL 12, 1979                   +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM D2$[8],D3$[10],G$[8],H$[2],T$[6],V$[8],V0$[30],X$[3]
0090 ON ESC THEN GOTO 0120
0100 ESC
0110 GOTO 0210
0120 ON ERR THEN GOTO 0140
0130 CLOSE FILE[3]
0140 ON ERR THEN GOTO 0160
0150 CLOSE FILE[0]
0160 ON ERR THEN STOP
0170 NOESC
0180 CHAIN "GC00"
0190 REM   ------------------------------------------------------------
0200 REM            COUNT IDENTIFIERS IN METHOD FILE
0210 READ FILE[4,1],T$
0220 CLOSE FILE[4]
0230 OPEN FILE[4],T$,200
0240 LET F=0
0250 READ FILE[4,3*(F+1)-1],V$
0260 IF EOF(4) THEN GOTO 0310
0270 LET F=F+1
0280 GOTO 0250
0290 REM   ------------------------------------------------------------
0300 REM            OPEN DATA FILE FOR DUPLICATE FIRST MEMBER
0310 PRINT
0320 ON ERR THEN GOTO 0340
0330 INPUT "WHAT IS THE INJECTION ID FOR THE FIRST MEMBER?  ",D2$
0340 ON ERR THEN STOP
0350 IF LEN(D2$)=8 THEN GOTO 0390
0360 PRINT
0370 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0380 GOTO 0310
0390 LET D3$="GC",D2$
0400 ON ERR THEN GOTO 0420
0410 RENAME D3$,D3$
0420 ON ERR THEN STOP

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                     PROGRAM LISTING FOR GC16

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0430 IF SYS(7)=-9 THEN GOTO 0470
0440 PRINT
0450 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0460 GOTO 0310
0470 ON ERR THEN GOTO 0510
0480 OPEN FILE[3,0],D3$,31
0490 ON ERR THEN STOP
0500 GOTO 0560
0510 ON ERR THEN STOP
0520 DELAY =1
0530 GOTO 0470
0540 REM   ------------------------------------------------------------
0550 REM           CHECK DATA FILE USABILITY AND PROCESSING FLAGS
0560 READ FILE[3,1],J,D3$,J2
0570 IF J=1 THEN GOTO 0660
0580 PRINT
0590 IF J<>2 THEN GOTO 0630
0600 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
0610 PRINT "     HAVE A TOTAL AREA"
0620 GOTO 1960
0630 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
0640 PRINT "     IN THE WRONG FORMAT."
0650 GOTO 1960
0660 IF J2=1 THEN GOTO 0730
0670 PRINT
0680 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SPIKED SAMPLE CALCULATION
*    S UNTIL"
0690 PRINT "     AFTER IT IS PROCESSED."
0700 GOTO 0120
0710 REM   ------------------------------------------------------------
0720 REM           FIND FIRST AND LAST ENTRIES IN DATA FILE
0730 LET P9=2
0740 READ FILE[3,P9],V0$
0750 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0780
0760 LET P9=P9+1
0770 GOTO 0740
0780 LET P9=P9+2
0790 LET P8=P9
0800 READ FILE[3,P8],G$
0810 IF EOF(3) THEN GOTO 0840
0820 LET P8=P8+1
0830 GOTO 0800

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0840 LET P8=P8-1
0850 REM   -------------------------------------------------------------
0860 REM            OPEN DATA FILE FOR DUPLICATE SECOND MEMBER
0870 PRINT
0880 ON ERR THEN GOTO 0900
0890 INPUT "WHAT IS THE INJECTION ID FOR THE SECOND MEMBER?  ",D2$
0900 ON ERR THEN STOP
0910 IF LEN(D2$)=8 THEN GOTO 0950
0920 PRINT
0930 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0940 GOTO 0870
0950 LET D3$="GC",D2$
0960 ON ERR THEN GOTO 0980
0970 RENAME D3$,D3$
0980 ON ERR THEN STOP
0990 IF SYS(7)=-9 THEN GOTO 1030
1000 PRINT
1010 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
1020 GOTO 0870
1030 ON ERR THEN GOTO 1070
1040 OPEN FILE[0,0],D3$,31
1050 ON ERR THEN STOP
1060 GOTO 1120
1070 ON ERR THEN STOP
1080 DELAY =1
1090 GOTO 1030
1100 REM   -------------------------------------------------------------
1110 REM            CHECK DATA FILE USABILITY AND PROCESSING FLAGS
1120 READ FILE[0,1],J,D3$,J2
1130 IF J=1 THEN GOTO 1220
1140 PRINT
1150 IF J<>2 THEN GOTO 1190
1160 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
1170 PRINT "     HAVE A TOTAL AREA"
1180 GOTO 1960
1190 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
1200 PRINT "     IN THE WRONG FORMAT."
1210 GOTO 1960
1220 IF J2=1 THEN GOTO 1290
1230 PRINT
1240 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SPIKED SAMPLE CALCULATION
*    S UNTIL"

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1250 PRINT "     AFTER IT IS PROCESSED."
1260 GOTO 0120
1270 REM   -------------------------------------------------------------
1280 REM            FIND FIRST AND LAST ENTRIES IN DATA FILE
1290 LET P7=2
1300 READ FILE[0,P7],V0$
1310 IF V0$[1,7]<>"MESSAGE" THEN GOTO 1340
1320 LET P7=P7+1
1330 GOTO 1300
1340 LET P7=P7+2
1350 LET P6=P7
1360 READ FILE[0,P6],G$
1370 IF EOF(0) THEN GOTO 1400
1380 LET P6=P6+1
1390 GOTO 1360
1400 LET P6=P6-1
1410 REM   -------------------------------------------------------------
1420 REM            PRINT HEADINGS
1430 PRINT
1440 PRINT
1450 PRINT  TAB(13);"D-U-P-L-I-C-A-T-E   S-A-M-P-L-E-S   R-E-P-O-R-T"
1460 READ FILE[3,1],J,D3$,J2
1470 PRINT "INJECTION ID FOR FIRST MEMBER:  ";D3$[3,10]; TAB(53);"METH
*    OD NUMBER:  ";T$[3,6]
1480 READ FILE[0,1],J,D3$,J2
1490 PRINT "INJECTION ID FOR SECOND MEMBER:  ";D3$[3,10]
1500 PRINT "CONCENTRATIONS IN MICROGRAMS/LITER"
1510 PRINT
1520 PRINT "                FIRST          SECOND         ABSOLUTE"
1530 PRINT "IDENTIFIER  CONCENTRATION  CONCENTRATION  DIFFERENCE"
1540 PRINT "----------  -------------  -------------  ----------"
1550 REM   -------------------------------------------------------------
1560 REM            FILL IN CHART
1570 FOR I=1 TO F
1580   READ FILE[4,3*I-1],V$
1590   IF V$="99999" THEN GOTO 1910
1600   FOR I2=P9 TO P8
1610     READ FILE[3,I2],G$,H$,B,C,L,L2
1620     IF G$=V$ THEN GOTO 1660
1630   NEXT I2
1640   LET C=-9999
1650   LET L=-9999

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1660    FOR I2=P7 TO P6
1670      READ FILE[0,I2],G$,H$,B,C2,L3,L2
1680      IF G$=V$ THEN GOTO 1720
1690    NEXT I2
1700    LET C2=-9999
1710    LET L3=-9999
1720    PRINT USING " ########   ",V$;
1730     IF C<>-9999 THEN GOTO 1760
1740    PRINT " NOT DETECTED  ";
1750    GOTO 1800
1760    IF L<>-9999 THEN GOTO 1790
1770    PRINT "NOT CALCULATED ";
1780    GOTO 1800
1790    PRINT USING "-----#.###     ",L;
1800    IF C2<>-9999 THEN GOTO 1830
1810    PRINT " NOT DETECTED  ";
1820    GOTO 1870
1830    IF L3<>-9999 THEN GOTO 1860
1840    PRINT "NOT CALCULATED ";
1850    GOTO 1870
1860    PRINT USING "-----#.###     ",L3;
1870    IF C<>-9999 THEN IF L<>-9999 THEN IF C2<>-9999 THEN IF L3<>-999
*     9 THEN GOTO 1900
1880    PRINT
1890    GOTO 1910
1900    PRINT USING " ++++#.###",L-L3
1910 NEXT I
1920 PRINT
1930 PRINT
1940 REM   ------------------------------------------------------------
1950 REM           WRAP-UP PROCEDURE
1960 ON ERR THEN GOTO 1980
1970 CLOSE FILE[3]
1980 ON ERR THEN GOTO 2000
1990 CLOSE FILE[0]
2000 ON ERR THEN STOP
2010 PRINT
2020 ON ERR THEN GOTO 2040
2030 INPUT "DO YOU WANT A REPORT FOR ANOTHER DUPLICATE PAIR?  (Y OR N)
*        ",X$
2040 ON ERR THEN STOP
2050 IF X$[1,1]="Y" THEN GOTO 0310

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
2060 NOESC
2070 CHAIN "GC00"

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  7
                         SYMBOL TABLE FOR GC16

SYMBOL    REFERENCES
------  -----------------------------------------------------------------
 0120   0090  0700  1260
 0140   0120
 0160   0140
 0210   0110
 0250   0280
 0310   0260  0380  0460  2050
 0340   0320
 0390   0350
 0420   0400
 0470   0430  0530
 0510   0470
 0560   0500
 0630   0590
 0660   0570
 0730   0660
 0740   0770
 0780   0750
 0800   0830
 0840   0810
 0870   0940  1020
 0900   0880
 0950   0910
 0980   0960
 1030   0990  1090
 1070   1030
 1120   1060
 1190   1150
 1220   1130
 1290   1220
 1300   1330
 1340   1310
 1360   1390
 1400   1370
 1660   1620
 1720   1680
 1760   1730
 1790   1760
 1800   1750  1780
 1830   1800
 1860   1830
 1870   1320  1850
 1900   1870
 1910   1590  1890
 1960   0620  0650  1180  1210
 1980   1960
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                       PAGE  8
                         SYMBOL TABLE FOR GC16

SYMBOL    REFERENCES
------  -----------------------------------------------------------------
 2000   1980
 2040   2020
 B      1610  1670
 C      1610  1640  1730  1870
 C2     1670  1700  1800  1870
 D2$    0080  0330  0350  0370  0390  0450  0600  0630  0680  0890
        0910  0930  0950  1010  1160  1190  1240
 D3$    0080  0390  0410  0480  0560  0950  0970  1040  1120  1460
        1470  1480  1490
 F      0240  0250  0270  1570
 FL#0   0150  1040  1120  1300  1360  1480  1670  1990
 FL#3   0130  0480  0560  0740  0800  1460  1610  1970
 FL#4   0210  0220  0230  0250  1580
 G$     0080  0800  1360  1610  1620  1670  1680
 H$     0080  1610  1670
 I      1570  1580  1910
 I2     1600  1610  1630  1660  1670  1690
 J      0560  0570  0590  1120  1130  1150  1460  1480
 J2     0560  0660  1120  1220  1460  1480
 L      1610  1650  1760  1790  1870  1900
 L2     1610  1670
 L3     1670  1710  1830  1860  1870  1900
 P6     1350  1360  1380  1400  1660
 P7     1290  1300  1320  1340  1350  1660
 P8     0790  0800  0820  0840  1600
 P9     0730  0740  0760  0780  0790  1600
 T$     0080  0210  0230  1470
 V$     0080  0250  1580  1590  1620  1680  1720
 VO$    0080  0740  0750  1300  1310
 X$     0080  2030  2050
```

SECTION 19

PROGRAM GC17 - SURROGATE SPIKES CALCULATION

GC17 is the program which calculates the percent recovery of surrogate spikes and prints a report. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

As GC27 begins, the method file is already open, and the program counts the number of identifiers in that file. It then asks the user for the injection ID for the sample containing the surrogate spike and opens the corresponding injection data file. The program then asks for the identifier of the surrogate spike compound. It searches the method file to be sure that the identifier is in the method, and then searches the data file to see if the compound was detected. It then asks the user for the prepared concentration of the surrogate spike, and prints the report.

Finally, the program closes the data file and asks the user if it should start over. It then either branches back to the beginning or chains back to GC00. The percent recovery of surrogate spikes is calculated by the formula:

$$\text{Percent Recovery} = 100 \bullet \frac{\text{Measured Concentration}}{\text{Prepared Concentration}}$$

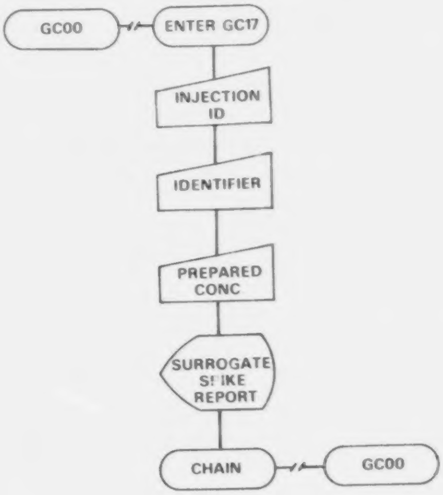


Figure 15. Flowchart of Program GC17.

TABLE 13. SYMBOL DEFINITIONS FOR PROGRAM GC17

A5	the prepared concentration of the surrogate spike
B	the absolute retention time
C	the peak area
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
J	the data file useablility flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 has been proccessed J2=2 never processed
L	the calculated concentration
L2	the relative retention time or capacity ratio
P9	the record number for the first peak in the data file
T$	the name of the method file
V$	the identifier from the method file
VO$	an error MESSAGE
V1$	the full chemical name of the surrogate spike compound

TABLE 13. (Continued)

V7$	the identifier input by the user
X$	the user's answer to Y or N questions

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                      PROGRAM LISTING FOR GC17

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                 +
0030 REM   +   PROGRAM GC17, SURROGATE SPIKE CALCULATIONS           +
0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 12, 1979               +
0050 REM   +   MOST RECENT REVISION:  APRIL 12, 1979                +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM D2$[8],D3$[10],G$[8],H$[2],T$[6],V$[8],V0$[30],V1$[40],V7$[8]
*    ,X$[3]
0090 ON ESC THEN GOTO 0120
0100 ESC
0110 GOTO 0190
0120 ON ERR THEN GOTO 0140
0130 CLOSE FILE[3]
0140 ON ERR THEN STOP
0150 NOESC
0160 CHAIN "GC00"
0170 REM  -------------------------------------------------------
0180 REM          COUNT IDENTIFIERS IN METHOD FILE
0190 READ FILE[4,1],T$
0200 CLOSE FILE[4]
0210 OPEN FILE[4],T$,200
0220 LET F=0
0230 READ FILE[4,3*(F+1)-1],V$
0240 IF EOF(4) THEN GOTO 0290
0250 LET F=F+1
0260 GOTO 0230
0270 REM  -------------------------------------------------------
0280 REM          OPEN DATA FILE
0290 PRINT
0300 ON ERR THEN GOTO 0320
0310 INPUT "WHAT IS THE INJECTION ID FOR THE SURROGATE SPIKE?  ",D2$
0320 ON ERR THEN STOP
0330 IF LEN(D2$)=8 THEN GOTO 0370
0340 PRINT
0350 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0360 GOTO 0290
0370 LET D3$="GC",D2$
0380 ON ERR THEN GOTO 0400
0390 RENAMF D3$,D3$
0400 ON ERR THEN STOP
0410 IF SYS(7)=-9 THEN GOTO 0450

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                      PROGRAM LISTING FOR GC17

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0420 PRINT
0430 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0440 GOTO 0290
0450 ON ERR THEN GOTO 0490
0460 OPEN FILE[3,0],D3$,31
0470 ON ERR THEN STOP
0480 GOTO 0540
0490 ON ERR THEN STOP
0500 DELAY =1
0510 GOTO 0450
0520 REM  ---------------------------------------------------------------
0530 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
0540 READ FILE[3,1],J,D3$,J2
0550 IF J=1 THEN GOTO 0640
0560 PRINT
0570 IF J<>2 THEN GOTO 0610
0580 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
0590 PRINT "     HAVE A TOTAL AREA"
0600 GOTO 1210
0610 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
0620 PRINT "     IN THE WRONG FORMAT."
0630 GOTO 1210
0640 IF J2=1 THEN GOTO 0710
0650 PRINT
0660 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SURROGATE SPIKE CALCULATI
*    ONS UNTIL"
0670 PRINT "     AFTER IT IS PROCESSED."
0680 GOTO 0120
0690 REM  ---------------------------------------------------------------
0700 REM          LOCATE DATA
0710 PRINT
0720 ON ERR THEN GOTO 0740
0730 INPUT "WHAT IS THE IDENTIFIER FOR THE SURROGATE SPIKE COMPOUND?
*    ",V7$
0740 ON ERR THEN STOP
0750 FOR I=1 TO F
0760   READ FILE[4,3*I-1],V$,V1$
0770   IF V$=V7$ THEN GOTO 0820
0780 NEXT I
0790 PRINT
0800 PRINT "<7><7>THERE IS NO IDENTIFIER ";V7$;" IN METHOD ";T$[3,6];"
*    ."

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE  3
                    PROGRAM LISTING FOR GC17

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0810 GOTO 1210
 0820 LET P9=2
 0830 READ FILE[3,P9],V0$
 0840 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0870
 0850 LET P9=P9+1
 0860 GOTO 0830
 0870 LET P9=P9+2
 0880 READ FILE[3,P9],G$,H$,B,C,L,L2
 0890 IF EOF(3)<>1 THEN GOTO 0930
 0900 PRINT
 0910 PRINT "<7><7>IDENTIFIER ";V7$;" WAS NOT DETECTED IN INJECTION ";D
*     2$;"."
 0920 GOTO 1210
 0930 IF G$=V7$ THEN GOTO 0960
 0940 LET P9=P9+1
 0950 GOTO 0880
 0960 IF C=-9999 THEN GOTO 0900
 0970 IF L<>-9999 THEN GOTO 1010
 0980 PRINT
 0990 PRINT "<7><7>THE CONCENTRATION OF ";D2$;" WAS NOT CALCULATED DURI
*     NG PROCESSING."
 1000 GOTO 1210
 1010 PRINT
 1020 PRINT "WHAT IS THE PREPARED CONCENTRATION OF ";V7$;" IN";
 1030 ON ERR THEN GOTO 1050
 1040 INPUT " MICROGRAMS/LITER?  ",A5
 1050 ON ERR THEN STOP
 1060 REM   ---------------------------------------------------------
 1070 REM          PRINT REPORT
 1080 PRINT
 1090 PRINT
 1100 PRINT  TAB(15);"S-U-R-R-O-G-A-T-E   S-P-I-K-E   R-E-P-O-R-T"
 1110 PRINT "INJECTION ID:  ";D2$; TAB(54);"METHOD NUMBER:  ";T$[3,6]
 1120 PRINT "PREPARED CONCENTRATION OF ";V1$;":  ";
 1130 PRINT USING "----#.###",A5
 1140 PRINT USING "CALCULATED CONCENTRATION:  -----#.###",L
 1150 PRINT USING "PERCENT RECOVERED:  ---#.#%",L/A5*100
 1160 PRINT "CONCENTRATIONS IN MICROGRAMS/LITER"
 1170 PRINT
 1180 PRINT
 1190 REM   ---------------------------------------------------------
 1200 REM          WRAP-UP PROCEDURE

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE  4
                    PROGRAM LISTING FOR GC17

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 1210 ON ERR THEN GOTO 1230
 1220 CLOSE FILE[3]
 1230 ON ERR THEN STOP
 1240 PRINT
 1250 ON ERR THEN GOTO 1270
 1260 INPUT "DO YOU WANT A REPORT ON ANOTHER SURROGATE SPIKE?  (Y OR N)
*     ",X$
 1270 ON ERR THEN STOP
 1280 IF X$[1,1]="Y" THEN GOTO 0290
 1290 NOESC
 1300 CHAIN "GC00"

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                 PAGE  5
                       SYMBOL TABLE FOR GC17

SYMBOL   REFERENCES
------   -----------------------------------------------------------------

 0120   0090  0680
 0140   0120
 0190   0110
 0230   0260
 0290   0240  0360  0440  1280
 0320   0300
 0370   0330
 0400   0380
 0450   0410  0510
 0490   0450
 0540   0480
 0610   0570
 0640   0550
 0710   0640
 0740   0720
 0820   0770
 0830   0860
 0870   0840
 0880   0950
 0900   0960
 0930   0890
 0960   0930
 1010   0970
 1050   1030
 1210   0600  0630  0810  0920  1000
 1230   1210
 1270   1250
 A5     1040  1130  1150
 B      0880
 C      0880  0960
 D2$    0080  0310  0330  0350  0370  0430  0580  0610  0660  0910
        0990  1110
 D3$    0080  0370  0390  0460  0540
 F      0220  0230  0250  0750
 FL#3   0130  0460  0540  0830  0880  1220
 FL#4   0190  0200  0210  0230  0760
 G$     0080  0880  0930
 H$     0080  0890
 I      0750  0760  0780
 J      0540  0550  0570
 J2     0540  0640
 L      0880  0970  1140  1150
 L2     0880
 P9     0820  0830  0850  0870  0880  0940
 T$     0080  0190  0210  0800  1110
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                 PAGE  6
                       SYMBOL TABLE FOR GC17

SYMBOL   REFERENCES
------   -----------------------------------------------------------------

 V$     0080  0230  0760  0770
 V0$    0080  0830  0840
 V1$    0080  0760  1120
 V7$    0080  0730  0770  0800  0910  0930  1020
 X$     0080  1260  1280
```

SECTION 20

PROGRAM GC18 - REPLICATE STATISTICS CALCULATION

GC18 is the program which calculates replicate statistics and prints a report. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

When GC18 begins, the method file is already open, and the program counts the number of identifiers in that file. The program then asks the user for the injection ID for a sample, and opens the corresponding injection data file. The program then reads each identifier from the method file and locates the calculated concentration of each identifier in the data file. It places the concentration in array O, and then it closes the data file and goes back to ask the user for another injection ID.

When the user types "END" as an injection ID (or when ten replicates have been entered) the program begins to print the report. It prints the headings first, and then fills in the table. It reads the replicate concentrations for each identifier from array O, calculates the mean concentration and standard deviation, and prints these statistics.

When all of the identifiers have been dealt with, the program asks the user if it should start over. It then either branches back to the beginning or chains back to GC00.

TABLE 14. SYMBOL DEFINITIONS FOR PROGRAM GC18

B	the absolute retention time
C	the peak area
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I$	the superstring of injection ID numbers for replicates
I2	the control variable for loops
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 never processed J2=2 processed
L	the calculated concentration
L2	the relative retention time or capacity ratio
O()	the array of calculated concentrations of replicates
P8	the record number for the last peak in the data file
P9	the record number for the first peak in the data file
R4	the standard deviation

TABLE 14. (Continued)

R5	the average concentration (arithmetic mean)
R6	the number of replicate injections
R7	the number of replicates of an individual compound
R8	the sum of the measured concentrations (used in calculating the average and the standard deviation)
R9	the sum of the squares of the measured concentrations (used in calculating the standard deviation)
T$	the name of the method file
V$	the identifier from the method file
VO$	an error MESSAGE
X$	the user's response to a Y or N question

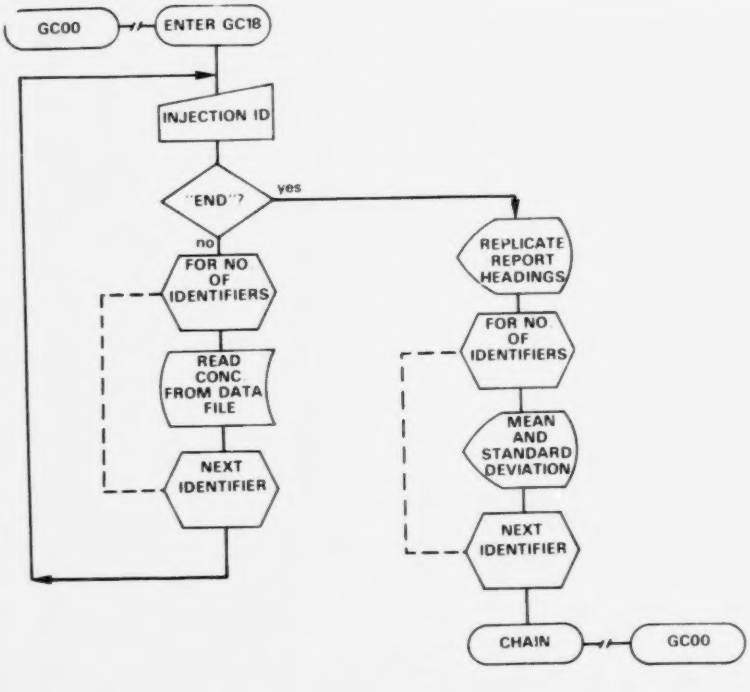

GC00
ENTER GC18
INJECTION ID
"END"?
yes
no
FOR NO OF IDENTIFIERS
READ CONC FROM DATA FILE
NEXT IDENTIFIER
REPLICATE REPORT HEADINGS
FOR NO. OF IDENTIFIERS
MEAN AND STANDARD DEVIATION
NEXT IDENTIFIER
CHAIN
GC00

Figure 16. Flowchart of Program GC18.

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                        PAGE  1
                       PROGRAM LISTING FOR GC18

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
 0030 REM   +   PROGRAM GC18, REPLICATE STATISTICS CALCULATIONS         +
 0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 16, 1979                  +
 0050 REM   +   MOST RECENT REVISION:  APRIL 16, 1979                   +
 0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0070 REM
 0080 DIM D2$[8],D3$[10],G$[8],H$[2],I$[80],O[60,10],T$[6],V$[8],V0$[30
*      ],X$[3]
 0090 ON ESC THEN GOTO 0120
 0100 ESC
 0110 GOTO 0190
 0120 ON ERR THEN GOTO 0140
 0130 CLOSE FILE[3]
 0140 ON ERR THEN STOP
 0150 NOESC
 0160 CHAIN "GC00"
 0170 REM   ------------------------------------------------------------
 0180 REM          COUNT IDENTIFIERS IN METHOD FILE
 0190 READ FILE[4,1],T$
 0200 CLOSE FILE[4]
 0210 OPEN FILE[4],T$,200
 0220 LET F=0
 0230 READ FILE[4,3*(F+1)-1],V$
 0240 IF EOF(4) THEN GOTO 0290
 0250 LET F=F+1
 0260 GOTO 0230
 0270 REM   ------------------------------------------------------------
 0280 REM          OPEN DATA FILE
 0290 PRINT
 0300 PRINT "ENTER THE INJECTION ID NUMBERS FOR THE REPLICATE INJECTION
*      S."
 0310 PRINT "TYPE 'END' TO TERMINATE THE LIST."
 0320 LET R6=0
 0330 LET I$=""
 0340 PRINT
 0350 IF R6<10 THEN GOTO 0390
 0360 PRINT "<7><7>YOU HAVE ENTERED TEN REPLICATES, WHICH IS THE LIMIT
*      "
 0370 PRINT "     FOR THIS PROGRAM."
 0380 GOTO 1140
 0390 ON ERR THEN GOTO 0410

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                        PAGE  2
                       PROGRAM LISTING FOR GC18

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0400 INPUT "INJECTION ID FOR REPLICATE?  ",D2$
 0410 ON ERR THEN STOP
 0420 IF D2$="END" THEN GOTO 1140
 0430 IF LEN(D2$)=8 THEN GOTO 0470
 0440 PRINT
 0450 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
 0460 GOTO 0340
 0470 LET D3$="GC",D2$
 0480 ON ERR THEN GOTO 0500
 0490 RENAME D3$,D3$
 0500 ON ERR THEN STOP
 0510 IF SYS(7)=-9 THEN GOTO 0550
 0520 PRINT
 0530 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
 0540 GOTO 0340
 0550 ON ERR THEN GOTO 0590
 0560 OPEN FILE[3,0],D3$,31
 0570 ON ERR THEN STOP
 0580 GOTO 0640
 0590 ON ERR THEN STOP
 0600 DELAY =1
 0610 GOTO 0550
 0620 REM   ------------------------------------------------------------
 0630 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
 0640 READ FILE[3,1],J,D3$,J2
 0650 IF J=1 THEN GOTO 0760
 0660 PRINT
 0670 IF J<>2 THEN GOTO 0720
 0680 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
 0690 PRINT "     HAVE A TOTAL AREA"
 0700 CLOSE FILE[3]
 0710 GOTO 0340
 0720 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
 0730 PRINT "     IN THE WRONG FORMAT."
 0740 CLOSE FILE[3]
 0750 GOTO 0340
 0760 IF J2=1 THEN GOTO 0840
 0770 PRINT
 0780 PRINT "<7><7>";D2$;" CANNOT BE USED FOR REPLICATE STATISTICS CALC
*      ULATIONS UNTIL"
 0790 PRINT "     AFTER IT IS PROCESSED."
 0800 CLOSE FILE[3]

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE  3
                       PROGRAM LISTING FOR GC18

1234567891123456789212345678931234567894123456789512345673961234567897
         0         0         0         0         0         0         0
0810 GOTO 0340
0820 REM   -----------------------------------------------------------
0830 REM           FIND FIRST AND LAST ENTRIES IN DATA FILE
0840 LET P9=2
0850 READ FILE[3,P9],V0$
0860 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0890
0870 LET P9=P9+1
0880 GOTO 0850
0890 LET P9=P9+2
0900 LET P8=P9
0910 READ FILE[3,P8],G$
0920 IF EOF(3) THEN GOTO 0950
0930 LET P8=P8+1
0940 GOTO 0910
0950 LET P8=P8-1
0960 REM   -----------------------------------------------------------
0970 REM           COPY DATA TO ARRAY
0980 LET R6=R6+1
0990 LET I$=I$,D2$
1000 FOR I=1 TO F
1010   READ FILE[4,3*I-1],V$
1020   FOR I2=P9 TO P8
1030     READ FILE[3,I2],G$,H$,B,C,L,L2
1040     IF G$=V$ THEN GOTO 1080
1050   NEXT I2
1060   LET O[I,R6]=-9999
1070   GOTO 1090
1080   LET O[I,R6]=L
1090 NEXT I
1100 CLOSE FILE[3]
1110 GOTO 0340
1120 REM   -----------------------------------------------------------
1130 REM           PRINT HEADING
1140 IF R6>1 THEN GOTO 1190
1150 PRINT
1160 PRINT "<7><7>REPLICATE STATISTICS CANNOT BE CALCULATED WITH FEWER
*      THAN"
1170 PRINT "     TWO GOOD INJECTIONS."
1180 GOTO 1660
1190 PRINT
1200 PRINT
1210 PRINT  TAB(10);"R-E-P-L-I-C-A-T-E   S-T-A-T-I-S-T-I-C-S   R-E-P-O
*      -R-T"

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE  4
                       PROGRAM LISTING FOR GC18

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1220 PRINT "METHOD NUMBER:  ";T$[3,6]; TAB(39);"CONCENTRATIONS IN MICR
*      OGRAMS/LITER"
1230 PRINT "REPLICATE INJECTION ID NUMBERS:  ";
1240 FOR I=1 TO R6
1250   PRINT I$[8*I-7,8*I];
1260   IF I<>R6 THEN PRINT ", ";
1270   IF I<>4 THEN GOTO 1300
1280   PRINT
1290   PRINT "      ";
1300 NEXT I
1310 PRINT
1320 PRINT
1330 PRINT "                AVERAGE       STANDARD   NUMBER OF"
1340 PRINT "IDENTIFIER  CONCENTRATION  DEVIATION  REPLICATES"
1350 PRINT "----------  -------------  ---------  ----------"
1360 REM   -----------------------------------------------------------
1370 REM           FILL IN CHART
1380 FOR I=1 TO F
1390   READ FILE[4,3*I-1],V$
1400   IF V$="99999" THEN GOTO 1620
1410   LET R8=0
1420   LET R9=0
1430   LET R7=0
1440   FOR I2=1 TO R6
1450     IF O[I,I2]=-9999 THEN GOTO 1490
1460     LET R7=R7+1
1470     LET R8=R8+O[I,I2]
1480     LET R9=R9+O[I,I2]^2
1490   NEXT I2
1500   PRINT USING " ######## ",V$;
1510   IF R7>0 THEN GOTO 1540
1520   PRINT "                                 0"
1530   GOTO 1620
1540   LET R5=R8/R7
1550   PRINT USING "  -----#.###   ",R5;
1560   IF R7>1 THEN GOTO 1590
1570   PRINT "           ";
1580   GOTO 1610
1590   LET R4=SQR((R9-R8^2/R7)/(R7-1))
1600   PRINT USING " -----#.## ",R4;
1610   PRINT USING "     ###",R7
1620 NEXT I

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  5
                    PROGRAM LISTING FOR GC18

 12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
 1630 REM   --------------------------------------------------------
 1640 REM          WRAP-UP PROCEDURE
 1650 PRINT
 1660 PRINT
 1670 ON ERR THEN GOTO 1690
 1680 INPUT "DO YOU WANT A REPORT ON ANOTHER SET OF REPLICATES?  (Y OR
*      N)  ",X$
 1690 ON ERR THEN STOP
 1700 IF X$[1,1]="Y" THEN GOTO 0290
 1710 NOESC
 1720 CHAIN "GC00"

 12345678911234567892123456789312345678941234567895123456789612345678970
          0          0          0          0          0          0          0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                    PAGE  6
                         SYMBOL TABLE FOR GC18

SYMBOL    REFERENCES
------  -----------------------------------------------------------------
 0120   0090
 0140   0120
 0190   0110
 0230   0260
 0290   0240  1700
 0340   0460  0540  0710  0750  0810  1110
 0390   0350
 0410   0390
 0470   0430
 0500   0480
 0550   0510  0610
 0590   0550
 0640   0580
 0720   0670
 0760   0650
 0840   0760
 0850   0880
 0890   0860
 0910   0940
 0950   0920
 1080   1040
 1090   1070
 1140   0380  0420
 1190   1140
 1300   1270
 1490   1450
 1540   1510
 1590   1560
 1610   1580
 1620   1400  1530
 1660   1180
 1690   1670
 B      1030
 C      1030
 D2$    0080  0400  0420  0430  0450  0470  0530  0680  0720  0780
        0990
 D3$    0080  0470  0490  0560  0640
 F      0220  0230  0250  1000  1380
 FL#3   0130  0560  0640  0700  0740  0800  0850  0910  1030  1100
 FL#4   0190  0200  0210  0230  1010  1390
 G$     0080  0910  1030  1040
 H$     0080  1030
 I      1000  1010  1060  1080  1090  1240  1250  1260  1270  1300
        1380  1390  1450  1470  1480  1620
 I$     0080  0330  0990  1250
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  7
                        SYMBOL TABLE FOR GC18

SYMBOL    REFERENCES
------  ----------------------------------------------------------------
  I2    1020  1030  1050  1440  1450  1470  1480  1490
  J     0640  0650  0670
  J2    0640  0760
  L     1030  1080
  L2    1030
  O[    0080  1060  1080  1450  1470  1480
  P8    0900  0910  0930  0950  1020
  P9    0840  0850  0870  0890  0900  1020
  R4    1590  1600
  R5    1540  1550
  R6    0320  0350  0980  1060  1080  1140  1240  1260  1440
  R7    1430  1460  1510  1540  1560  1590  1610
  R8    1410  1470  1540  1590
  R9    1420  1480  1590
  T$    0080  0190  0210  1220
  V$    0080  0230  1010  1040  1390  1400  1500
  V0$   0080  0850  0860
  X$    0080  1680  1700
```

SECTION 21

PROGRAM GC19 - DISSIMILAR ANALYSIS CONFIRMATION

GC19 is the program which prints a dissimilar analysis confirmation report. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

GC19 first asks the user for the method numbers and the injection ID numbers to be used in the confirmation report. The user is forced to input at least two but no more than four method numbers and at least one but no more than four injection ID numbers for each of the methods. The method numbers and injection ID numbers are checked as they are input to ensure that they are valid numbers and that the corresponding data files exist. The names of the method files are placed in superstring S5$, and the names of the data files are placed in superstring S6$.

The program then asks the user for the identifier for which the confirmation report is to be compiled, and it checks to be sure that the identifier does occur in all of the specified methods.

Next, the program prints the headings for the report, and then begins to fill in the report. For each line of the report, the program opens a data file and locates the concentration for the specified identifier.

When the report is complete, the program asks the user whether it should start over. If the user answers YES, the program branches back to the point of asking for the identifier to be used. Otherwise, control is returned to GC00.

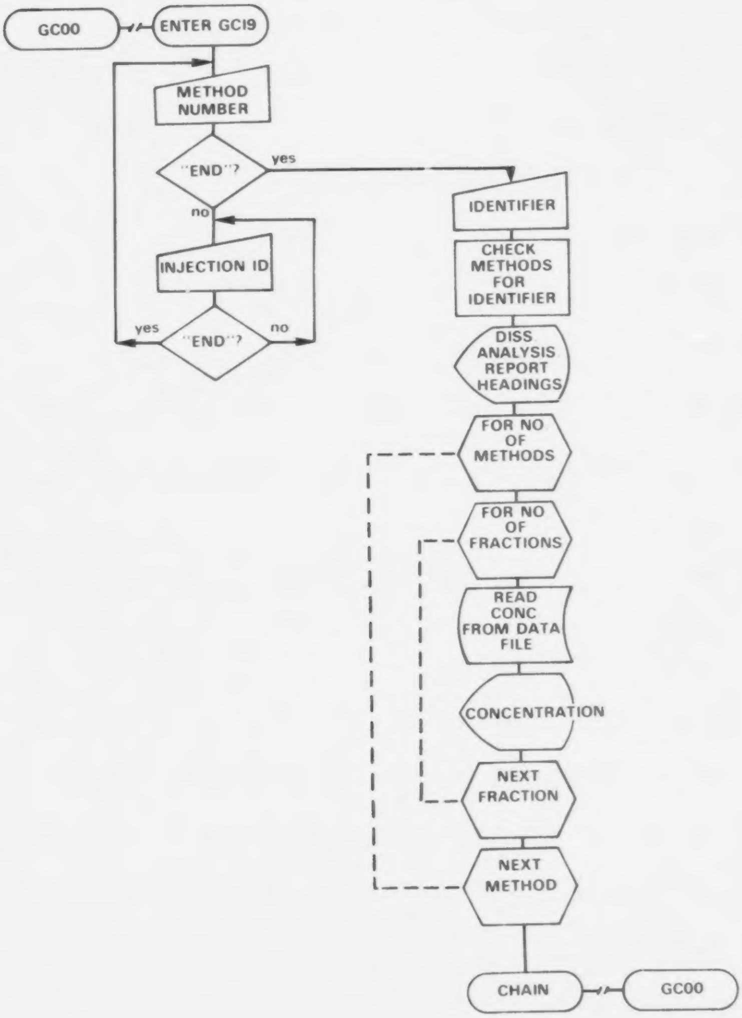

GC00
ENTER GC19
METHOD NUMBER
"END"?
yes
no
INJECTION ID
"END"?
yes
no
IDENTIFIER
CHECK METHODS FOR IDENTIFIER
DISS ANALYSIS REPORT HEADINGS
FOR NO OF METHODS
FOR NO OF FRACTIONS
READ CONC FROM DATA FILE
CONCENTRATION
NEXT FRACTION
NEXT METHOD
CHAIN
GC00

Figure 17. Flowchart of Program GC19.

TABLE 15. SYMBOL DEFINITIONS FOR PROGRAM GC19

B	the absolute retention time
C	the peak area
D2$	the injection ID
D3$	the name of a data file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I2	the control variable for loops
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 processed J2=2 never processed
L	the calculated concentration
P9	the record number being accessed in the data file
S5	the counter for the number of methods
S5$	the superstring of the names of the method files
S6$	the superstring of the names of the data files
S6()	the array of four counters which count the number of data files used with each method
S7	the record number being accessed in the method file
T	the method number

TABLE 15. (Continued)

T$	the name of the method file
T1$	the method number as a string
V$	the identifier from the method file
V0$	an error MESSAGE from the data file
V7$	the identifier for which the report is generated
X$	the user's response to a Y or N question
Z5	the character position of a slash in the identifier

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                       PROGRAM LISTING FOR GC19

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0010 REM    +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0020 REM    +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                  +
 0030 REM    +   PROGRAM GC19, DISSIMILAR ANALYSIS CONFIRMATION        +
 0040 REM    +   BY:  J. KOPKE (SWORCC), APRIL 19, 1979                +
 0050 REM    +   MOST RECENT REVISION:  APRIL 19, 1979                 +
 0060 REM    +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0070 REM
 0080 ON ESC THEN GOTO 2040
 0090 ESC
 0100 DIM D2$[8],D3$[10],G$[8],H$[2],S5$[24],S6$[160],S6[4],T$[6],T1$[6
*     ],V$[8],V0$[30],V7$[8],X$[3]
 0110 REM    ------------------------------------------------------------
 0120 REM              INPUT METHOD NUMBERS
 0130 LET S5$="                        "
 0140 FOR I=1 TO 16
 0150   LET S6$=S6$,"          "
 0160 NEXT I
 0170 LET S5=0
 0180 IF S5<>4 THEN GOTO 0190
 0182 PRINT
 0184 PRINT "<7><7>YOU HAVE ENTERED FOUR METHODS WHICH IS THE LIMIT FOR
*      THIS PROGRAM."
 0186 GOTO 0940
 0190 PRINT
 0200 PRINT "WHAT IS THE NUMBER OF THE ";
 0210 ON S5+1 THEN GOTO 0220, 0240, 0260, 0280
 0220 PRINT "FIRST ";
 0230 GOTO 0290
 0240 PRINT "SECOND ";
 0250 GOTO 0290
 0260 PRINT "THIRD ";
 0270 GOTO 0290
 0280 PRINT "FOURTH ";
 0290 PRINT "METHOD?"
 0300 ON ERR THEN GOTO 0320
 0310 INPUT "     (TYPE 'END' TO TERMINATE THE LIST OF METHODS)  ",T1$
 0320 ON ERR THEN STOP
 0330 IF T1$<>"END" THEN GOTO 0380
 0340 IF S5>1 THEN GOTO 0940
 0350 PRINT
 0360 PRINT "<7><7>YOU MUST USE AT LEAST TWO DIFFERENT METHODS."
 0370 GOTO 0190

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                       PROGRAM LISTING FOR GC19

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0380 ON ERR THEN GOTO 0420
 0390 LET T=VAL(T1$)
 0400 ON ERR THEN STOP
 0410 IF T=ABS(INT(T)) THEN IF T>0 THEN IF T<10000 THEN GOTO 0460
 0420 ON ERR THFN STOP
 0430 PRINT
 0440 PRINT "<7><7>";T1$;" IS NOT A VALID METHOD NUMBER."
 0450 GOTO 0190
 0460 LET T$="GC0000"
 0470 LET T$[7-LEN(STR$(T)),6]=STR$(T)
 0480 ON ERR THEN GOTO 0500
 0490 RENAME T$,T$
 0500 ON ERR THEN STOP
 0510 IF SYS(7)<>-10 THEN GOTO 0550
 0520 PRINT
 0530 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*     ];"."
 0540 GOTO 0190
 0550 PRINT
 0560 LET S5=S5+1
 0570 LET S5$[6*S5-5,6*S5]=T$
 0580 REM    ------------------------------------------------------------
 0590 REM              INPUT INJECTION ID NUMBERS
 0600 LET S6[S5]=0
 0610 IF S6[S5]<>4 THEN GOTO 0620
 0612 PRINT "<7><7>YOU HAVE ENTERED FOUR FRACTIONS WHICH IS THE LIMIT F
*     OR ONE METHOD."
 0614 GOTO 0180
 0620 PRINT "WHAT IS THE INJECTION ID FOR THE ";
 0630 ON S6[S5]+1 THEN GOTO 0640, 0660, 0680, 0700
 0640 PRINT "FIRST ";
 0650 GOTO 0710
 0660 PRINT "SECOND ";
 0670 GOTO 0710
 0680 PRINT "THIRD ";
 0690 GOTO 0710
 0700 PRINT "FOURTH ";
 0710 PRINT "FRACTION FOR METHOD ";T$[3,6];"?"
 0720 ON ERR THEN GOTO 0740
 0730 INPUT "     (TYPE 'END' TO TERMINATE THE LIST OF FRACTIONS)  ",D2
*     $
 0740 ON ERR THEN STOP

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE  3
                      PROGRAM LISTING FOR GC19

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0750 IF D2$<>"END" THEN GOTO 0790
0760 IF S6[S5]>0 THEN GOTO 0180
0770 PRINT "<7><7>YOU MUST USE AT LEAST ONE FRACTION FOR A METHOD."
0780 GOTO 0620
0790 IF LEN(D2$)=8 THEN GOTO 0820
0800 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID NUMBER."
0810 GOTO 0620
0820 LET D3$="GC",D2$
0830 ON ERR THEN GOTO 0850
0840 RENAME D3$,D3$
0850 ON ERR THEN STOP
0860 IF SYS(7)<>-10 THEN GOTO 0890
0870 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ";D2$;"."
0880 GOTO 0620
0890 LET S6[S5]=S6[S5]+1
0900 LET S6$[((S5-1)*40)+S6[S5]*10-9,((S5-1)*40)+S6[S5]*10]=D3$
0910 GOTO 0610
0920 REM  -----------------------------------------------------------
0930 REM            CHECK METHOD FOR PRESENCE OF IDENTIFIER
0940 PRINT
0950 ON ERR THEN GOTO 0990
0960 INPUT "WHAT IS THE IDENTIFIER FOR WHICH YOU WANT A CONFIRMATION R
*     EPORT?  ",V7$
0970 ON ERR THEN STOP
0980 GOTO 1030
0990 ON ERR THEN STOP
1000 PRINT
1010 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
1020 GOTO 0940
1030 LET Z5=POS(V7$,"/",1)
1040 IF 75=0 THFN GOTO 1070
1050 LET V7$[Z5,Z5]=","
1060 GOTO 1030
1070 FOR I=1 TO S5
1080    ON ERR THEN GOTO 1120
1090    OPEN FILE[4,0],S5$[6*I-5,6*I],200
1100    ON ERR THEN STOP
1110    GOTO 1160
1120    PRINT
1130    PRINT "<7><7>METHOD ";S5$[6*I-3,6*I];" IS BEING USED BY ANOTHER
*     USER."
1140    PRINT "     THIS OPTION IS BEING TERMINATED."

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE  4
                      PROGRAM LISTING FOR GC19

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1150    GOTO 2040
1160    LET S7=1
1170    READ FILE[4,3*S7-1],V$
1180    IF EOF(4)<>1 THEN GOTO 1230
1190    PRINT
1200    PRINT "<7><7>IDENTIFIER ";V7$;" DOES NOT APPEAR IN METHOD ";S5$
*     [6*I-3,6*I];"."
1210    CLOSE
1220    GOTO 1980
1230    IF V$=V7$ THEN GOTO 1260
1240    LET S7=S7+1
1250    GOTO 1170
1260    CLOSE
1270 NEXT I
1280 REM  ------------------------------------------------------------
1290 REM            PRINT HEADINGS
1300 PRINT
1310 PRINT
1320 PRINT "     D-I-S-S-I-M-I-L-A-R   A-N-A-L-Y-S-I-S   C-O-N-F-I-R-M
*     -A-T-I-O-N"
1330 PRINT "IDENTIFIER:  ";V7$; TAB(39);"CONCENTRATIONS IN MICROGRAMS/
*     LITER"
1340 PRINT
1350 PRINT "METHOD  INJECTION   CALCULATED"
1360 PRINT "NUMBER     ID       CONCENTRATION"
1370 PRINT "------  ---------   -------------"
1380 REM  ------------------------------------------------------------
1390 REM          FILL IN CHART
1400 FOR I=1 TO S5
1410    FOR I2=1 TO S6[I]
1420       LET D3$=S6$[((I-1)*40)+I2*10-9,((I-1)*40)+I2*10]
1430       ON ERR THEN GOTO 1470
1440       OPEN FILE[3,0],D3$,31
1450       ON ERR THEN STOP
1460       GOTO 1520
1470       ON ERR THEN STOP
1480       PRINT
1490       PRINT "<7><7>THE DATA FOR INJECTION ";D3$;" IS BEING USED BY
*     ANOTHER USER."
1500       PRINT "     THIS OPTION IS BEING TERMINATED."
1510       GOTO 2040
1520       REM  -------------------------------------

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
       0         0         0         0         0         0         0
1530     REM     CHECK DATA FILE FLAGS
1540     READ FILE[3,1],J,D3$,J2
1550     IF J=1 THEN GOTO 1640
1560     PRINT
1570     IF J<>2 THEN GOTO 1610
1580     PRINT "<7><7>";D3$[3,10];" CANNOT BE USED BECAUSE THE REPORT
*     DID NOT HAVE"
1590     PRINT "      A TOTAL AREA.  ";
1600     GOTO 1670
1610     PRINT "<7><7>";D3$;" CANNOT BE USED BECAUSE THE REPORT WAS IN
*     THE WRONG"
1620     PRINT "      FORMAT.  ";
1630     GOTO 1670
1640     IF J2=1 THEN GOTO 1710
1650     PRINT "<7><7>";D3$[3,10];" CANNOT RE USED FOR DISSIMILAR ANAL
*     YSIS CONFIRMATION"
1660     PRINT "     UNTIL AFTER IT IS PROCESSED.  ";
1670     PRINT "THIS OPTION IS BEING TERMINATED."
1680     GOTO 2040
1690     REM   ---------------------------------------
1700     REM     FIND CONCENTRATION
1710     LET P9=2
1720     READ FILE[3,P9],V0$
1730     IF V0$[1,7]<>"MESSAGE" THEN GOTO 1760
1740     LET P9=P9+1
1750     GOTO 1720
1760     LET P9=P9+2
1770     READ FILE[3,P9],G$,H$,B,C,L
1780     IF EOF(3)<>1 THEN GOTO 1800
1790     LET C=-9999
1800     IF G$=V7$ THEN GOTO 1830
1810     LET P9=P9+1
1820     GOTO 1770
1830     CLOSE
1840     PRINT USING " ####    ########",S5$[6*I-3,6*I],D3$[3,10];
1850     IF C<>-9999 THEN GOTO 1880
1860     PRINT "   NOT DETECTED"
1870     GOTO 1920
1880     IF L<>-9999 THEN GOTO 1910
1890     PRINT "  NOT CALCULATED"
1900     GOTO 1920
1910     PRINT USING "  -----#.###",L

1234567891123456789212345678931234567894123456789512345678961234567897
       0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
       0         0         0         0         0         0         0
1920   NEXT I2
1930   PRINT
1940 NEXT I
1950 REM   ------------------------------------------------------------
1960 REM          WRAP-UP PROCEDURE
1970 PRINT
1980 PRINT
1990 ON ERR THEN GOTO 2020
2000 PRINT "DO YOU WANT A CONFIRMATION REPORT FOR ANOTHER COMPOUND USI
*    NG"
2010 INPUT "     THE SAME METHODS AND FRACTIONS?  (Y OR N)  ",X$
2020 ON ERR THEN STOP
2030 IF X$[1,1]="Y" THEN GOTO 0940
2040 CLOSE
2050 NOESC
2060 CHAIN "GC00" THEN GOTO 0100

1234567891123456789212345678931234567894123456789512345678961234567897
       0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  7
                     SYMBOL TABLE FOR GC19

SYMBOL   REFERENCES
------  ------------------------------------------------------------
 0100   2060
 0180   0614  0760
 0190   0180  0370  0450  0540
 0220   0210
 0240   0210
 0260   0210
 0280   0210
 0290   0230  0250  0270
 0320   0300
 0380   0330
 0420   0380
 0460   0410
 0500   0480
 0550   0510
 0610   0910
 0620   0610  0780  0810  0880
 0640   0630
 0660   0630
 0680   0630
 0700   0630
 0710   0650  0670  0690
 0740   0720
 0790   0750
 0820   0790
 0850   0830
 0890   0860
 0940   0186  0340  1020  2030
 0990   0950
 1030   0980  1060
 1070   1040
 1120   1080
 1160   1110
 1170   1250
 1230   1180
 1260   1230
 1470   1430
 1520   1460
 1610   1570
 1640   1550
 1670   1600  1630
 1710   1640
 1720   1750
 1760   1730
 1770   1820
 1800   1780
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  8
                     SYMBOL TABLE FOR GC19

SYMBOL   REFERENCES
------  ------------------------------------------------------------
 1830   1800
 1880   1850
 1910   1880
 1920   1870  1900
 1980   1220
 2020   1990
 2040   0080  1150  1510  1680
 B      1770
 C      1770  1790  1850
 D2$    0100  0730  0750  0790  0800  0820  0870
 D3$    0100  0820  0840  0900  1420  1440  1490  1540  1580  1610
        1650  1840
 FL#3   1440  1540  1720  1770
 FL#4   1090  1170
 G$     0100  1770  1800
 H$     0100  1770
 I      0140  0160  1070  1090  1130  1200  1270  1400  1410  1420
        1840  1940
 I2     1410  1420  1920
 J      1540  1550  1570
 J2     1540  1640
 L      1770  1880  1910
 P9     1710  1720  1740  1760  1770  1810
 S5     0170  0180  0210  0340  0560  0570  0600  0610  0630  0760
        0890  0900  1070  1400
 S5$    0100  0130  0570  1090  1130  1200  1840
 S6$    0100  0150  0900  1420
 S6[    0100  0600  0610  0630  0760  0890  0900  1410
 S7     1160  1170  1240
 T      0390  0410  0470
 T$     0100  0460  0470  0490  0530  0570  0710
 T1$    0100  0310  0330  0390  0440
 V$     0100  1170  1230
 V0$    0100  1720  1730
 V7$    0100  0960  1030  1050  1200  1230  1330  1800
 X$     0100  2010  2030
 Z5     1030  1040  1050
```

SECTION 22

PROGRAM GC20 - SAMPLE FILE CONTROL INTERACTION

GC20 is the module of the GCAS which creates run results files for transmission to the Sample File Control (SFC) System. The format of the run results file is defined in the document "EPA Sample File Control Functional Design." The program is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed. Also, if the escape key is pressed, the run results file being created is deleted.

As GC20 begins, it gives the user the choice of creating a new run results file, editing an existing run results file, or sending an existing run results file to the SFC computer. If the user chooses to edit a file, control is passed to the SFC foreground BASIC program RUNEDIT. Similarly, if the user wants to send a run results file to the SFC computer, control is passed to the program SEND.

If the user chooses to create a new run results file, GC20 asks for the information necessary to name the file and generate its header record.

Next, the program allows the user to report any laboratory control standards. The user must enter the injection ID and concentration pattern letter for each control standard, and the program copies the appropriate data from the injection data file and concentration pattern file into the run results file.

The user is then allowed to report the concentrations of samples to SFC, along with any combination of spikes, duplicates, and surrogate spikes. The user enters the injection ID for the sample, and the calculated concentrations are copied from the injection data file into the run results file. The prepared concentration of any surrogate spike is also placed in the run results file. For a spiked sample, the user enters the injection ID for the sample after spiking and the concentration pattern for the spike added values, and the program copies the appropriate data from the injection data file and concentration pattern file into the run results file. Again, the prepared concentration of any surrogate spike is also placed into the run results file. For a duplicate of a sample, the user enters the injection ID for the duplicate, and the program copies the necessary data from the injection ID file into the run results file. Once again, the prepared concentration of any surrogate spike is also placed into the run results file.

When the user has placed all of the data for a set of samples into the run results file, the program forces the user to use either RUNEDIT or SEND. When either of these programs is completed, control is returned to the GCAS master control program, GCOO.

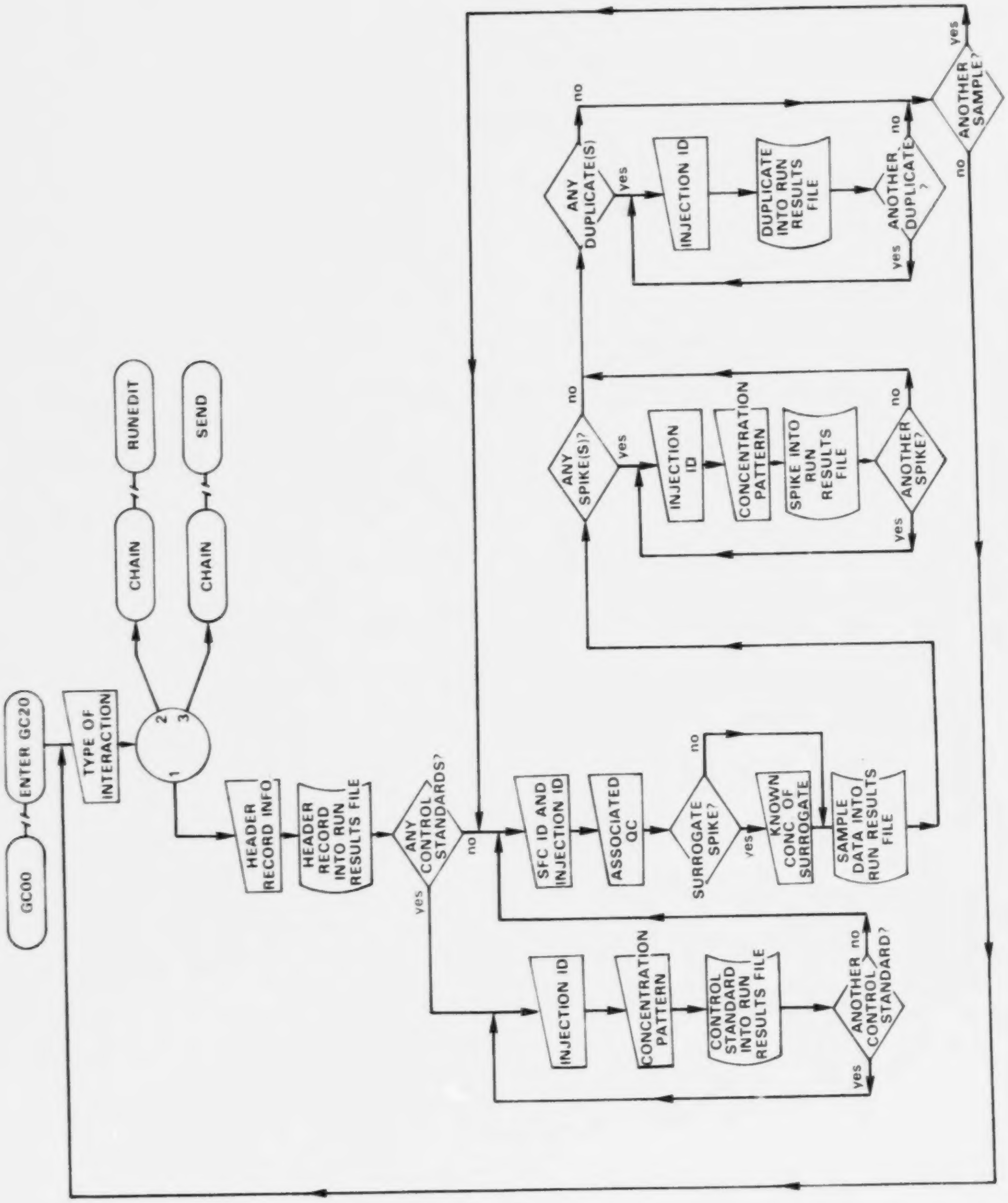

GC00
ENTER GC20
TYPE OF INTERACTION
1
2
3
CHAIN
RUNEDIT
CHAIN
SEND
HEADER RECORD INFO
HEADER RECORD INTO RUN RESULTS FILE
ANY CONTROL STANDARDS?
yes
no
INJECTION ID
CONCENTRATION PATTERN
CONTROL STANDARD INTO RUN RESULTS FILE
ANOTHER CONTROL STANDARD?
yes
no
SFC ID AND INJECTION ID
ASSOCIATED QC
SURROGATE SPIKE?
yes
no
KNOWN CONC OF SURROGATE
SAMPLE DATA INTO RUN RESULTS FILE
ANY SPIKE(S)?
yes
no
INJECTION ID
CONCENTRATION PATTERN
SPIKE INTO RUN RESULTS FILE
ANOTHER SPIKE?
yes
no
ANY DUPLICATE(S)
yes
no
INJECTION ID
DUPLICATE INTO RUN RESULTS FILE
ANOTHER DUPLICATE ?
yes
no
ANOTHER SAMPLE?
yes
no

Figure 18. Flowchart of Program GC20.

TABLE 16. SYMBOL DEFINITIONS FOR PROGRAM GC20

A5	the concentration from a concentration pattern file
A6$	the name of a concentration pattern file
A7	the position of A8$ in A9$
A8$	the letter name of a concentration pattern
A9$	the alphabet
B	the absolute retention time
C	the peak area
D2$	an injection ID number
D3$	the name of an injection data file
E9	a flag which is used by subroutines to report to the main program that the current process should be terminated E9=0 continue normally E9=1 terminate process
F	the number of identifiers in the method file
G$	an identifier from an injection data file
H$	the peak type
I	the control variable for loops
I2	the control variable for loops
I8$	the measurement instrument ID
I9$	the initials of the analyst
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format

TABLE 16. (Continued)

J2	the data file processing flag J2=1 has been processed J2=2 never processed
L	the calculated concentration
N7$	the non-numeric result code
N8$	the QC type code
N9$	the QC type code for duplicates
P8	the record number of the last peak in the injection data file
P9	the record number of the first peak in the injection data file
Q5$	the format for PRINT USING statements
Q6$	the format for PRINT USING statements
R$	the name of the run results file
R1$	the parameter/method code
S9$	the identifier for the surrogate spike compound
T$	the name of the method file
T9$	the SFC sample ID number
V$	an identifier for the surrogate spike compound
V0$	a MESSAGE read from a data file
V1$	the full name of the first compound associated with an identifier
V2$	the CAS number for V1$
V3$	the full name of the second compound associated with an identifier
W3$	a CAS number with the hyphens removed
X	the user's answer to multiple choice questions
X$	the user's answer to most Y OR N questions

TABLE 16. (Continued)

X1$	the user's answer to a Y OR N question
X2$	the user's answer to a Y OR N question
X3$	the user's answer to a Y OR N question
X4	the prepared concentration of a surrogate spike
X4$	the user's answer to a Y OR N question
Z9	a counter for the number of spikes or duplicates of a sample

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE  1
                       PROGRAM LISTING FOR GC20

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
 0030 REM   +   PROGRAM GC20, SAMPLE FILE CONTROL INTERACTION            +
 0040 REM   +   BY:  J. KOPKE (SWORCC), MAY 25, 1979                    +
 0050 REM   +   MOST RECENT REVISION:  MAY 29, 1979                     +
 0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
 0070 REM
 0080 DIM A6$[9],A8$[1],A9$[26],D2$[8],D3$[10],G$[8],H$[2],I8$[5],I9$[3
*     ],N7$[3]
 0090 DIM N8$[3],N9$[3],Q5$[80],Q6$[80],R$[11],R1$[7],S9$[8],T$[6],T9$[
*     8],V$[8]
 0100 DIM V0$[30],V1$[40],V2$[11],V3$[40],W3$[9],X$[1],X1$[1],X2$[1],X3
*     $[1],X4$[1]
 0110 LET Q5$="2 ######## ### C ########## #.####^^^^ UG/L     ###
*
 0120 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
 0130 UN ESC THEN GOTO 0370
 0140 ESC
 0150 REM   --------------------------------------------------------------
 0160 REM             CHECK VALIDITY OF THE METHOD FOR SFC PURPOSES
 0170 READ FILE[4,1],T$
 0180 CLOSE FILE[4]
 0190 OPEN FILE[4],T$,200
 0200 LET F=0
 0210 READ FILE[4,3*(F+1)-1],V$,V1$,V2$,V3$
 0220 IF EOF(4) THEN GOTO 0520
 0230 IF V3$="99999" THEN GOTO 0280
 0240 PRINT
 0250 PRINT "<7><7>METHOD ";T$[3,6];" CANNOT BE USED FOR SFC PURPOSES B
*     ECAUSE "
 0260 PRINT "     IT DEALS WITH CO-ELUTING COMPOUNDS."
 0270 GOTO 0370
 0280 IF LEN(V2$)<>0 THEN GOTO 0330
 0290 PRINT
 0300 PRINT "<7><7>METHOD ";T$[3,6];" CANNOT BE USED FOR SFC PURPOSES B
*     ECAUSE"
 0310 PRINT "     IT IS MISSING AT LEAST ONE CAS NUMBER."
 0320 GOTO 0370
 0330 LET F=F+1
 0340 GOTO 0210
 0350 REM   --------------------------------------------------------------
 0360 REM             ABNORMAL ENDING ROUTINE

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                   PAGE  2
                       PROGRAM LISTING FOR GC20

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
 0370 ON ERR THEN GOTO 0390
 0380 CLOSE FILE[0]
 0390 ON ERR THEN GOTO 0410
 0400 CLOSE FILE[3]
 0410 ON ERR THEN GOTO 0430
 0420 CLOSE FILE[7]
 0430 ON ERR THEN GOTO 0470
 0440 DELETE R$
 0450 PRINT
 0460 PRINT "<7><7>THE RUN RESULTS FILE HAS BEEN DELETED BECAUSE IT WAS
*       INCOMPLETE."
 0470 ON ERR THEN STOP
 0430 NOESC
 0490 CHAIN "GC00"
 0500 REM   --------------------------------------------------------------
 0510 REM             INPUT TYPE OF INTERACTION
 0520 PRINT
 0530 PRINT "HERE ARE THE TYPES OF SAMPLE FILE CONTROL INTERACTION:"
 0540 PRINT
 0550 PRINT "     1.  CREATE A NEW RUN RESULTS FILE"
 0560 PRINT "     2.  EDIT OR DELETE AN EXISTING RUN RESULTS FILE"
 0570 PRINT "     3.  SEND AN EXISTING RUN RESULTS FILE TO THE SFC COMP
*     UTER"
 0580 PRINT
 0590 ON ERR THEN GOTO 0610
 0600 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, OR 3)  ",X
 0610 ON ERR THEN STOP
 0620 IF X=INT(X) THEN IF X>0 THEN IF X<4 THEN GOTO 0660
 0630 PRINT
 0640 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
 0650 GOTO 0520
 0660 ON X THEN GOTO 0960, 0690, 0830
 0670 REM   --------------------------------------------------------------
 0680 REM             EDIT A RUN RESULTS FILE
 0690 PRINT
 0700 PRINT "YOU ARE BEING TRANSFERRED TO THE SFC 'RUNEDIT' PROGRAM WHI
*     CH"
 0710 PRINT "     WILL ALLOW YOU TO DELETE OR MODIFY YOUR RUN RESULTS F
*     ILE."
 0720 PRINT "AFTER YOU HAVE COMPLETED 'RUNEDIT' YOU WILL BE TRANSFERRED
*       BACK"
 0730 PRINT "     TO THIS SYSTEM."

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC20

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
 0740 PRINT "THEN, REMEMBER TO SEND THE RUN RESULTS FILE TO THE SFC COM
*      PUTER."
 0750 FOR I=1 TO 10
 0760   PRINT
 0770 NEXT I
 0780 NOESC
 0790 CLOSE
 0800 CHAIN "RUNEDIT"
 0810 REM   ----------------------------------------------------------
 0820 REM           SEND A RUN RESULTS FILE TO THE PDP-11
 0830 PRINT
 0840 PRINT "YOU ARE BEING TRANSFERRED TO THE SFC 'SEND' PROGRAM WHICH
*      WILL"
 0850 PRINT "     ALLOW YOU TO SEND YOUR RUN RESULTS FILE TO THE SFC CO
*      MPUTER."
 0860 PRINT "AFTER YOU HAVE FINISHED 'SEND' YOU WILL BE TRANSFERRED BAC
*      K TO"
 0870 PRINT "     THIS SYSTEM."
 0880 FOR I=1 TO 10
 0890   PRINT
 0900 NEXT I
 0910 NOESC
 0920 CLOSE
 0930 CHAIN "SEND"
 0940 REM   ----------------------------------------------------------
 0950 REM           OPEN RUN RESULTS FILE
 0960 PRINT
 0970 ON ERR THEN GOTO 0990
 0980 INPUT "WHAT IS THE PARAMETER/METHOD CODE FOR THE RUN?  ",R1$
 0990 ON ERR THEN STOP
 1000 LET I2=1
 1010 LET R$=R1$,A9$[I2,I2],".BJ"
 1020 ON ERR THEN GOTO 1040
 1030 RENAME R$,R$
 1040 ON ERR THEN STOP
 1050 IF SYS(7)<>-10 THEN GOTO 1120
 1060 LET R$=R1$,A9$[I2,I2],".RR"
 1070 ON ERR THEN GOTO 1090
 1080 RENAME R$,R$
 1090 ON ERR THEN STOP
 1100 IF SYS(7)<>-10 THEN GOTO 1120
 1110 GOTO 1190

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC20

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
 1120 LET I2=I2+1
 1130 IF I2<27 THEN GOTO 1010
 1140 PRINT
 1150 PRINT "<7><7>THERE ARE ALREADY 26 RUN RESULTS FILES FOR PARAMETER
*      /METHOD"
 1160 PRINT "     CODE ";R1$;"."
 1170 PRINT "REPORT THIS PROBLEM TO THE NOVA SYSTEM MANAGER."
 1180 GOTO 0370
 1190 OPEN FILE[0,1],R$
 1200 PRINT
 1210 ON ERR THEN GOTO 1230
 1220 INPUT "WHAT IS THE MEASUREMENT INSTRUMENT ID?  ",I8$
 1230 ON ERR THEN GOTO 1260
 1240 PRINT
 1250 INPUT "WHAT ARE THE INITIALS OF THE RESPONSIBLE ANALYST?  ",I9$
 1260 ON ERR THEN STOP
 1270 LET Q6$="1 ## ## ## ## ## ##### ####### ###
*                        "
 1280 PRINT FILE[0],USING Q6$,SYS(3)-1900,SYS(2),SYS(1),SYS(11),SYS(12)
*      ,I3$,R$,I9$
 1290 REM   ----------------------------------------------------------
 1300 REM           PUT CONTROL STANDARDS INTO RUN RESULTS FILE
 1310 PRINT
 1320 ON ERR THEN GOTO 1340
 1330 INPUT "DO YOU WANT TO REPORT ANY CONTROL STANDARD(S) TO SFC?  (Y
*      OR N)  ",X$
 1340 ON ERR THEN STOP
 1350 IF X$[1,1]<>"Y" THEN GOTO 1780
 1360 PRINT
 1370 ON ERR THEN GOTO 1390
 1380 INPUT "WHAT IS THE INJECTION ID FOR THE CONTROL STANDARD?  ",D2$
 1390 ON ERR THEN STOP
 1400 GOSUB 3820
 1410 IF E9<>0 THEN GOTO 1710
 1420 PRINT
 1430 ON ERR THEN GOTO 1450
 1440 INPUT "WHAT IS THE CONCENTRATION PATTERN FOR THE CONTROL STANDARD
*      ?  ",A8$
 1450 ON ERR THEN STOP
 1460 GOSUB 4440
 1470 IF E9<>0 THEN GOTO 1710
 1480 FOR I=1 TO F

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
        0         0         0         0         0         0         0
1490    LET N7$="   "
1500    READ FILE[4,3*I-1],V$,V1$,V2$
1510    IF V$="99999" THEN GOTO 1680
1520    READ FILE[7,I],A5
1530    FOR I2=P9 TO P8 STEP 1
1540      READ FILE[3,I2],G$,H$,B,C,L
1550      IF G$=V$ THEN GOTO 1580
1560    NEXT I2
1570    LET C=-9999
1580    IF C<>-9999 THEN GOTO 1620
1590    LET L=0
1600    LET N7$="BDL"
1610    GOTO 1650
1620    IF L<>-9999 THEN GOTO 1650
1630    LET L=0
1640    LET N7$="NAR"
1650    LET W3$=V2$[1,6],V2$[8,9],V2$[11]
1660    PRINT FILE[0],USING Q5$," ","LCM",W3$,L,N7$
1670    PRINT FILE[0],USING Q5$," ","LCT",W3$,A5," "
1680 NEXT I
1690 CLOSE FILE[3]
1700 CLOSE FILE[7]
1710 PRINT
1720 ON ERR THEN GOTO 1740
1730 INPUT "DO YOU WANT TO REPORT ANOTHER CONTROL STANDARD TO SFC?  ",
*    X$
1740 ON ERR THEN STOP
1750 IF X$[1,1]="Y" THEN GOTO 1360
1760 REM   ----------------------------------------------------------------
1770 REM          INPUT SURROGATE SPIKE IDENTIFIER
1780 PRINT
1790 ON ERR THEN GOTO 1810
1800 INPUT "DO YOU WANT TO REPORT ANY SAMPLE(S) BACK TO SFC?  (Y OR N)
*     ",X$
1810 ON ERR THEN STOP
1820 IF X$[1,1]<>"Y" THEN GOTO 3730
1830 PRINT
1840 ON ERR THEN GOTO 1860
1850 INPUT "HAVE YOU USED A SURROGATE SPIKE WITH ANY OF THE SAMPLES?
*     (Y OR N)  ",X1$
1860 ON ERR THEN STOP
1870 IF X1$[1,1]<>"Y" THEN GOTO 2010

1234567891123456789212345678931234567894123456789512345678961234567897
        0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
        0         0         0         0         0         0         0
1880 PRINT
1890 ON ERR THEN GOTO 1910
1900 INPUT "WHAT IS THE IDENTIFIER FOR THE SURROGATE SPIKE COMPOUND?
*     ",S9$
1910 ON ERR THEN STOP
1920 FOR I=1 TO F
1930   READ FILE[4,3*I-1],V$
1940   IF V$=S9$ THEN GOTO 2010
1950 NEXT I
1960 PRINT
1970 PRINT "<7><7>THERE IS NO SUCH IDENTIFIER IN METHOD ";T$[3,6];"."
1980 GOTO 1830
1990 REM   ----------------------------------------------------------------
2000 REM          INPUT INFORMATION FOR SAMPLE
2010 PRINT
2020 ON ERR THEN GOTO 2040
2030 INPUT "WHAT IS THE SFC SAMPLE ID FOR THE SAMPLE?  ",T9$
2040 ON ERR THEN GOTO 2070
2050 PRINT
2060 INPUT "WHAT IS THE CORRESPONDING INJECTION ID NUMBER?  ",D2$
2070 ON ERR THEN STOP
2080 GOSUB 3820
2090 IF E9<>0 THEN GOTO 3680
2100 PRINT
2110 ON ERR THEN GOTO 2130
2120 INPUT "DO YOU WANT TO REPORT ANY SPIKE(S) FOR THIS SAMPLE?  (Y OR
*     N)  ",X2$
2130 ON ERR THEN GOTO 2160
2140 PRINT
2150 INPUT "DO YOU WANT TO REPORT ANY DUPLICATE(S) FOR THIS SAMPLE?  (
*     Y OR N)  ",X3$
2160 ON ERR THEN STOP
2170 IF X1$[1,1]="Y" THEN GOTO 2200
2180 LET X4$="N"
2190 GOTO 2320
2200 PRINT
2210 PRINT "DID YOU ADD THE SURROGATE SPIKE ";S9$;
2220 ON ERR THEN GOTO 2240
2230 INPUT " TO THIS SAMPLE?  (Y OR N)  ",X4$
2240 ON ERR THEN STOP
2250 IF X4$[1,1]<>"Y" THEN GOTO 2320
2260 PRINT

1234567891123456789212345678931234567894123456789512345678961234567897
        0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  7
                      PROGRAM LISTING FOR GC20

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
 2270 ON ERR THEN GOTO 2290
 2280 INPUT "WHAT IS THE PREPARED CONCENTRATION OF THE SURROGATE SPIKE?
*      ",X4
 2290 ON ERR THEN STOP
 2300 REM  ------------------------------------------------------------
 2310 REM           PUT UNKNOWN INTO RUN RESULTS FILE
 2320 IF X2$[1,1]="Y" THEN GOTO 2380
 2330 IF X3$[1,1]="Y" THEN GOTO 2360
 2340 LET N8$="   "
 2350 GOTO 2420
 2360 LET N8$="LD1"
 2370 GOTO 2420
 2380 IF X3$[1,1]="Y" THEN GOTO 2410
 2390 LET N8$="LSO"
 2400 GOTO 2420
 2410 LET N8$="LDX"
 2420 FOR I=1 TO F
 2430   LET N7$="   "
 2440   READ FILE[4,3*I-1],V$,V1$,V2$
 2450   IF V$="99999" THEN GOTO 2650
 2460   FOR I2=P9 TO P8 STEP 1
 2470     READ FILE[3,I2],G$,H$,B,C,L
 2480     IF G$=V$ THEN GOTO 2510
 2490   NEXT I2
 2500   LET C=-9999
 2510   IF C<>-9999 THEN GOTO 2550
 2520   LET L=0
 2530   LET N7$="BDL"
 2540   GOTO 2580
 2550   IF L<>-9999 THEN GOTO 2580
 2560   LET L=0
 2570   LET N7$="NAR"
 2580   LET W3$=V2$[1,6],V2$[8,9],V2$[11]
 2590   IF X4$[1,1]<>"Y" THEN GOTO 2640
 2600   IF V$<>S9$ THEN GOTO 2640
 2610   PRINT FILE[0],USING Q5$,T9$,"LS1",W3$,L,N7$
 2620   PRINT FILE[0],USING Q5$,T9$,"LS2",W3$,X4," "
 2630   GOTO 2650
 2640   PRINT FILE[0],USING Q5$,T9$,N8$,W3$,L,N7$
 2650 NEXT I
 2660 CLOSE FILE[3]
 2670 REM  ------------------------------------------------------------

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  8
                      PROGRAM LISTING FOR GC20

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
 2680 REM           PUT SPIKE INTO RUN RESULTS FILE
 2690 IF X2$[1,1]<>"Y" THEN GOTO 3200
 2700 LET Z9=0
 2710 PRINT
 2720 ON ERR THEN GOTO 2740
 2730 INPUT "WHAT IS THE INJECTION ID OF THE SAMPLE AFTER SPIKING?  ",D
*      2$
 2740 ON ERR THEN STOP
 2750 GOSUB 3820
 2760 IF E9<>0 THEN GOTO 3120
 2770 PRINT
 2780 ON ERR THEN GOTO 2800
 2790 INPUT "WHAT IS THE CONCENTRATION PATTERN FOR THE SPIKE ADDED VALU
*      ES?  ",A8$
 2800 ON ERR THEN STOP
 2810 GOSUB 4440
 2820 IF E9<>0 THEN GOTO 3120
 2830 FOR I=1 TO F
 2840   LET N7$="   "
 2850   READ FILE[4,3*I-1],V$,V1$,V2$
 2860   IF V$="99999" THEN GOTO 3080
 2870   READ FILE[7,I],A5
 2880   FOR I2=P9 TO P8 STEP 1
 2890     READ FILE[3,I2],G$,H$,B,C,L
 2900     IF G$=V$ THEN GOTO 2930
 2910   NEXT I2
 2920   LET C=-9999
 2930   IF C<>-9999 THEN GOTO 2970
 2940   LET L=0
 2950   LET N7$="BDL"
 2960   GOTO 3000
 2970   IF L<>-9999 THEN GOTO 3000
 2980   LET L=0
 2990   LET N7$="NAR"
 3000   LET W3$=V2$[1,6],V2$[8,9],V2$[11]
 3010   IF X4$[1,1]<>"Y" THEN GOTO 3060
 3020   IF V$<>S9$ THEN GOTO 3060
 3030   PRINT FILE[0],USING Q5$,T9$,"LS1",W3$,L,N7$
 3040   PRINT FILE[0],USING Q5$,T9$,"LS2",W3$,X4+A5,"   "
 3050   GOTO 3080
 3060   PRINT FILE[0],USING Q5$,T9$,"LSF",W3$,L,N7$
 3070   PRINT FILE[0],USING Q5$,T9$,"LSA",W3$,A5,"   "

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
3080 NEXT I
3090 CLOSE FILE[3]
3100 CLOSE FILE[7]
3110 LET Z9=Z9+1
3120 IF Z9<1 THEN GOTO 2710
3130 PRINT
3140 ON ERR THEN GOTO 3160
3150 INPUT "DO YOU WANT TO REPORT ANOTHER SPIKE OF THE SAME SAMPLE?  (
*    Y OR N)  ",X$
3160 ON ERR THEN STOP
3170 IF X$[1,1]="Y" THEN GOTO 2710
3180 REM  --------------------------------------------------------------
3190 REM          PUT DUPLICATE INTO RUN RESULTS FILE
3200 IF X3$[1,1]<>"Y" THEN GOTO 3680
3210 LET Z9=0
3220 PRINT
3230 ON ERR THEN GOTO 3250
3240 INPUT "WHAT IS THE INJECTION ID FOR THE DUPLICATE OF THE SAMPLE?
*     ",D2$
3250 ON ERR THEN STOP
3260 GOSUB 3820
3270 IF E9<>0 THEN GOTO 3550
3280 LET N9$="LD",STR$(Z9+2)
3290 FOR I=1 TO F
3300   LET N7$="    "
3310   READ FILE[4,3*I-1],V$,V1$,V2$
3320   IF V$="99999" THEN GOTO 3520
3330   FOR I2=P9 TO P8 STEP 1
3340     READ FILE[3,I2],G$,H$,B,C,L
3350     IF G$=V$ THEN GOTO 3380
3360   NEXT I2
3370   LET C=-9999
3380   IF C<>-9999 THEN GOTO 3420
3390   LET L=0
3400   LET N7$="BDL"
3410   GOTO 3450
3420   IF L<>-9999 THEN GOTO 3450
3430   LET L=0
3440   LET N7$="NAR"
3450   LET W3$=V2$[1,6],V2$[8,9],V2$[11]
3460   IF X4$[1,1]<>"Y" THEN GOTO 3510
3470   IF V$<>S9$ THEN GOTO 3510

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
3480   PRINT FILE[0],USING Q5$,T9$,"LS1",W3$,L,N7$
3490   PRINT FILE[0],USING Q5$,T9$,"LS2",W3$,X4,"    "
3500   GOTO 3520
3510   PRINT FILE[0],USING Q5$,T9$,N9$,W3$,L,N7$
3520 NEXT I
3530 CLOSE FILE[3]
3540 LET Z9=Z9+1
3550 IF Z9<1 THEN GOTO 3220
3560 IF Z9<8 THEN GOTO 3610
3570 PRINT
3580 PRINT "YOU HAVE REPORTED EIGHT DUPLICATES FOR THIS SAMPLE, WHICH
*     IS"
3590 PRINT "      THE MAXIMUM ALLOWED BY SFC."
3600 GOTO 3680
3610 PRINT
3620 ON ERR THEN GOTO 3640
3630 INPUT "DO YOU WANT TO REPORT ANOTHER DUPLICATE OF THE SAME SAMPLE
*     ?  (Y OR N)  ",X$
3640 ON ERR THEN STOP
3650 IF X$[1,1]="Y" THEN GOTO 3220
3660 REM  --------------------------------------------------------------
3670 REM          WRAP-UP PROCEDURE
3680 PRINT
3690 ON ERR THEN GOTO 3710
3700 INPUT "DO YOU WANT TO REPORT ANOTHER SAMPLE TO SFC?  (Y OR N)  ",
*     X$
3710 ON ERR THEN STOP
3720 IF X$[1,1]="Y" THEN GOTO 2010
3730 CLOSE FILE[0]
3740 PRINT
3750 PRINT "THE NAME OF THE RUN RESULTS FILE IS '";R$[1,LEN(R$)-3];"'.
*     "
3760 LET R$=""
3770 PRINT
3780 PRINT "YOU MUST NOW EITHER DELETE THIS FILE OR SEND IT TO THE SFC
*      COMPUTER."
3790 GOTO 0520
3800 REM  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
3810 REM          SUBROUTINE TO OPEN DATA FILE
3820 IF LEN(D2$)=8 THEN GOTO 3870
3830 PRINT
3840 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                        PAGE 11
                         PROGRAM LISTING FOR GC20

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
3850 LET E9=1
3860 RETURN
3870 LET D3$="GC",D2$
3880 ON ERR THFN GOTO 3900
3890 RENAME D3$,D3$
3900 ON ERR THEN STOP
3910 IF SYS(7)=-9 THEN GOTO 3960
3920 PRINT
3930 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
3940 LET E9=1
3950 RETURN
3960 ON ERR THEN GOTO 4000
3970 OPEN FILE[3,0],D3$,31
3980 ON ERR THEN STOP
3990 GOTO 4050
4000 ON ERR THEN STOP
4010 DELAY =1
4020 GOTO 3960
4030 REM    -----------------------------------------------------------
4040 REM            CHECK DATA FILE USABILITY AND PROCESSING FLAGS
4050 READ FILE[3,1],J,D3$,J2
4060 IF J=1 THEN GOTO 4190
4070 PRINT
4080 IF J<>2 THEN GOTO 4140
4090 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
4100 PRINT "     HAVE A TOTAL AREA."
4110 CLOSE FILE[3]
4120 LET E9=1
4130 RETURN
4140 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
4150 PRINT "     IN THE WRONG FORMAT."
4160 CLOSE FILE[3]
4170 LET E9=1
4180 RETURN
4190 IF J2=1 THEN GOTO 4280
4200 PRINT
4210 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SFC PURPOSES UNTIL"
4220 PRINT "     AFTER IT IS PROCESSED."
4230 CLOSE FILE[3]
4240 LET E9=1
4250 RETURN
4260 REM    -----------------------------------------------------------

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                        PAGE 12
                         PROGRAM LISTING FOR GC20

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
4270 REM            FIND FIRST AND LAST ENTRIES IN DATA FILE
4280 LET P9=2
4290 READ FILE[3,P9],V0$
4300 IF V0$[1,7]<>"MESSAGE" THEN GOTO 4330
4310 LET P9=P9+1
4320 GOTO 4290
4330 LET P9=P9+2
4340 LET P8=P9
4350 READ FILE[3,P8],G$
4360 IF EOF(3) THEN GOTO 4390
4370 LET P8=P8+1
4380 GOTO 4350
4390 LET P8=P8-1
4400 LET E9=0
4410 RETURN
4420 REM    +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
4430 REM            SUBROUTINE TO OPEN CONCENTRATION PATTERN FILE
4440 LET A7=POS(A9$,A8$,1)
4450 IF A7<>0 THEN GOTO 4500
4460 PRINT
4470 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
4480 LET E9=1
4490 RETURN
4500 LET A6$=T$,"000"
4510 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
4520 ON ERR THEN GOTO 4540
4530 RENAME A6$,A6$
4540 ON ERR THEN STOP
4550 IF SYS(7)=-9 THEN GOTO 4610
4560 PRINT
4570 PRINT "<7><7>THERE IS NO EXISTING CONCENTRATION PATTERN NAMED '";
*    A8$;"'."
4580 CLOSE FILE[3]
4590 LET E9=1
4600 RETURN
4610 ON ERR THEN GOTO 4660
4620 OPEN FILE[7,0],A6$,4
4630 ON ERR THEN STOP
4640 LET E9=0
4650 RETURN
4660 ON ERR THEN STOP
4670 DELAY =1

 1234567891123456789212345678931234567894123456789512345678961234567897
          0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE 13
                    PROGRAM LISTING FOR GC20

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
4680 GOTO 4610




1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE 14
                         SYMBOL TABLE FOR GC20

SYMBOL   REFERENCES
------  -------------------------------------------------------------
 0210   0340
 0280   0230
 0330   0280
 0370   0130  0270  0320  1180
 0390   0370
 0410   0390
 0430   0410
 0470   0430
 0520   0220  0650  3790
 0610   0590
 0660   0620
 0690   0660
 0830   0660
 0960   0660
 0990   0970
 1010   1130
 1040   1020
 1090   1070
 1120   1050  1100
 1190   1110
 1230   1210
 1260   1230
 1340   1320
 1360   1750
 1390   1370
 1450   1430
 1580   1550
 1620   1580
 1650   1610  1620
 1680   1510
 1710   1410  1470
 1740   1720
 1780   1350
 1810   1790
 1830   1980
 1860   1840
 1910   1890
 2010   1870  1940  3720
 2040   2020
 2070   2040
 2130   2110
 2160   2130
 2200   2170
 2240   2220
 2290   2270
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE 15
                         SYMBOL TABLE FOR GC20

SYMBOL   REFERENCES
------  ---------------------------------------------------------------
 2320   2190  2250
 2360   2330
 2380   2320
 2410   2380
 2420   2350  2370  2400
 2510   2480
 2550   2510
 2580   2540  2550
 2640   2590  2600
 2650   2450  2630
 2710   3120  3170
 2740   2720
 2800   2780
 2930   2900
 2970   2930
 3000   2960  2970
 3060   3010  3020
 3080   2860  3050
 3120   2760  2820
 3160   3140
 3200   2690
 3220   3550  3650
 3250   3230
 3380   3350
 3420   3380
 3450   3410  3420
 3510   3460  3470
 3520   3320  3500
 3550   3270
 3610   3560
 3640   3620
 3680   2090  3200  3600
 3710   3690
 3730   1820
 3820   1400  2080  2750  3260
 3870   3820
 3900   3880
 3960   3910  4020
 4000   3960
 4050   3990
 4140   4080
 4190   4060
 4280   4190
 4290   4320
 4330   4300
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                       PAGE 16
                         SYMROL TABLE FOR GC20

SYMBOL   REFERENCES
------  ---------------------------------------------------------------
 4350   4380
 4390   4360
 4440   1460  2810
 4500   4450
 4540   4520
 4610   4550  4680
 4660   4610
 A5     1520  1670  2870  3040  3070
 A6$    0080  4500  4510  4530  4620
 A7     4440  4450  4510
 A8$    0080  1440  2790  4440  4470  4570
 A9$    0080  0120  1010  1060  4440
 B      1540  2470  2890  3340
 C      1540  1570  1580  2470  2500  2510  2890  2920  2930  3340
        3370  3380
 D2$    0080  1380  2060  2730  3240  3820  3840  3870  3930  4090
        4140  4210
 D3$    0080  3870  3890  3970  4050
 E9     1410  1470  2090  2760  2820  3270  3850  3940  4120  4170
        4240  4400  4480  4590  4640
 F      0200  0210  0330  1480  1920  2420  2830  3290
 FL#0   0380  1190  1280  1660  1670  2610  2620  2640  3030  3040
        3060  3070  3480  3490  3510  3730
 FL#3   0400  1540  1690  2470  2660  2890  3090  3340  3530  3970
        4050  4110  4160  4230  4290  4350  4580
 FL#4   0170  0180  0190  0210  1500  1930  2440  2850  3310
 FL#7   0420  1520  1700  2870  3100  4620
 G$     0080  1540  1550  2470  2480  2890  2900  3340  3350  4350
 H$     0080  1540  2470  2890  3340
 I      0750  0770  0880  0900  1480  1500  1520  1680  1920  1930
        1950  2420  2440  2650  2830  2850  2870  3080  3290  3310
        3520
 I2     1000  1010  1060  1120  1130  1530  1540  1560  2460  2470
        2490  2880  2890  2910  3330  3340  3360
 I8$    0080  1220  1280
 I9$    0080  1250  1280
 J      4050  4060  4080
 J2     4050  4190
 L      1540  1590  1620  1630  1660  2470  2520  2550  2560  2610
        2640  2890  2940  2970  2980  3030  3060  3340  3390  3420
        3430  3480  3510
 N7$    0080  1490  1600  1640  1660  2430  2530  2570  2610  2640
        2840  2950  2990  3030  3060  3300  3400  3440  3480  3510
 N8$    0090  2340  2360  2390  2410  2640
 N9$    0090  3280  3510
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE 17
                        SYMBOL TABLE FOR GC20

SYMBOL   REFERENCES
------   ------------------------------------------------------------
 P8      1530 2460 2880 3330 4340 4350 4370 4390
 P9      1530 2460 2880 3330 4280 4290 4310 4330 4340
 Q5$     0090 0110 1660 1670 2610 2620 2640 3030 3040 3060
         3070 3480 3490 3510
 Q6$     0090 1270 1280
 R$      0090 0440 1010 1030 1060 1080 1190 1280 3750 3760
 R1$     0090 0980 1010 1060 1160
 S9$     0090 1900 1940 2210 2600 3020 3470
 T$      0090 0170 0190 0250 0300 1970 4500
 T9$     0090 2030 2610 2620 2640 3030 3040 3060 3070 3480
         3490 3510
 V$      0090 0210 1500 1510 1550 1930 1940 2440 2450 2480
         2600 2850 2860 2900 3020 3310 3320 3350 3470
 V0$     0100 4290 4300
 V1$     0100 0210 1500 2440 2850 3310
 V2$     0100 0210 0280 1500 1650 2440 2580 2850 3000 3310
         3450
 V3$     0100 0210 0230
 W3$     0100 1650 1660 1670 2580 2610 2620 2640 3000 3030
         3040 3060 3070 3450 3480 3490 3510
 X       0600 0620 0640 0660
 X$      0100 1330 1350 1730 1750 1800 1820 3150 3170 3630
         3650 3700 3720
 X1$     0100 1850 1870 2170
 X2$     0100 2120 2320 2690
 X3$     0100 2150 2330 2380 3200
 X4      2280 2620 3040 3490
 X4$     0100 2180 2230 2250 2590 3010 3460
 Z9      2700 3110 3120 3210 3280 3540 3550 3560
```

SECTION 23

PROGRAM GC21 - MICROCOMPUTER INTERFACE

GC21 is the program to receive data from the microcomputer and compact it into an injection data file. The microcomputer copies a report as it is printed by the Varian. It then sends an escape character to the Nova and waits for the Nova to respond with "ACCOUNT ID." The microcomputer then sends the account ID to the Nova and waits for the Nova to respond with the asterisk prompt. The microcomputer then sends to the Nova the command RUN "GC21". When this program reaches the INPUT statement, it sends a question mark prompt to the microcomputer. The microcomputer then sends to the Nova one line of the Varian report followed by a carriage return, and the program places the line into the arrival file. This continues until the entire report has been transmitted. Then, instead of sending a line of a report, the microcomputer sends an escape character to the Nova. GC21 then generates the name of the data file, enters that name into the ID list file, and compacts the report into the data file. When GC21 terminates, the word STOP is sent by the Nova to the microcomputer, which then sends a BYE command back to the Nova, ending the session. Details for the functions of the microcomputer can be found in the EPA document "Intercomputer Communications Using Microprocessors."

All of the above would be a simple process, except for the fact that Varian reports can vary considerably. GC21 must be prepared to handle any possibility, since the microcomputer is unable to react to Nova error messages. Consequently, GC21 contains a variety of complicated procedures which may never be used. For example, before GC21 opens any file, it always sets the ON ERR THEN GOTO condition in case the file is in use or is being dumped to tape for some reason. If an error does occur in opening a file, GC21 waits one second and tries again.

GC21 is divided into three main sections: 1) a procedure to input the report from the microcomputer and store it in an arrival file, 2) a procedure to compact the report from the arrival file into an injection data file and store that name in the ID list file, and 3) a subroutine to name an injection data file.

FROM MICROCOMPUTER TO ARRIVAL FILE

The first procedure is to input the report from the microcomputer and store it in the arrival file. GC20 simply inputs a line of the report as a string variable. An ON ERR THEN GOTO condition is established for this INPUT statement in case an analyst uses a comma in the Varian report title.

If the line which is input has a length of zero, GC21 immediately returns to the INPUT statement.

Beginning with the second line of the Varian report, GC21 checks each line to see if it begins with the letters GC. Every Varian report should begin with the letters GC and end with the words TOTAL AREA. However, if for some reason a report does not end with TOTAL AREA, the microcomputer will not recognize the end of the report, and it will continue to transmit a second report as if it were a part of the first. For this reason, GC21 checks every line for the letters GC. If the line does not begin with GC, it is written into the arrival file, and the program branches back to the INPUT statement. However, if a line does begin with GC, the program branches to the subroutine to generate the name of the injection data file, and then places into that data file a flag (a "2") to indicate that the report is not useable. GC21 then reopens the arrival file and begins to copy the second report into it.

When an escape character is received instead of a line of a report, GC21 branches to the next routine.

FROM ARRIVAL FILE TO DATA FILE

When the arrival file is complete, GC21 branches to the subroutine to generate the name of the injection data file. Then the arrival file is scanned for the line.

PEAK NAME TYPE COMP RETN CORR AREA FACTOR.

If this line cannot be found, the Varian report is in the wrong format. In such a case, GC21 writes into the data file a flag (a "3") to indicate that the report is not useable, and then GC21 stops.

If the report is in the correct format, GC21 continues to scan the arrival file for the TOTAL AREA line, and records the total area. A flag (a "1") is written into the injection data file to indicate that the report is useable.

Next, GC21 begins to scan the arrival file a third time. It finds the method number and the report title, if any, and writes them into the injection data file.

Continuing its scan through the arrival file, GC21 locates the lines referring to individual peaks. It does this by attempting to convert the first six characters of each line to a number. Lines in which this cannot be done are error messages, second page headings, or total concentrations which should be ignored.

The peak identifier and peak type are recorded from each line of data. The retention time is converted to a number and recorded. The percent area is converted to a number, multiplied by the total area, and divided by 100 to find the actual area of the peak. These four items are then written into the injection data file.

When the entire arrival file has been scanned for the third time, GC21 stops.

SUBROUTINE TO NAME AN INJECTION DATA FILE

Generating the name of an injection data file really involves generating the injection ID number. To do this, the subroutine first scans the arrival file for the instrument number, which it uses to create the name of the appropriate ID list file. It then attempts to RENAME the ID list file with the same name. This always produces an error which is trapped by an ON ERR THEN GOTO statement. If the error number is -10, the ID list file already exists and can be used. If the error number is -9, the ID list file has not been created for the instrument. In this second case, the subroutine creates an ID list file and fills it with 100 dummy entries.

The subroutine then determines the date for the injection ID number. If the analyst has specified a date in the operator identification field of the Varian report, that date is used. (This feature allows the operator of an auto-injector to keep the date from changing at midnight.) Otherwise, the date from the Nova system clock is used.

Next, the subroutine assigns the sequence number for the injection. To do this, it must use the date and sequence number of the previous injection, which it finds in the first injection ID number in the ID list file. If the date of the current injection is the same as the date of the previous injection, the sequence number assigned is 1 greater than the previous sequence number. If the dates are different, the sequence number is reset to 01.

Finally the subroutine deletes the oldest data file in the ID list file. The ON ERR THEN GOTO condition is again set for this DELETE statement because the oldest ID number in the file may be a dummy entry. All of the other ID numbers (data files names) are shifted down one position in the ID list file, and the newest ID is placed at the top of the list. Control is then returned to the invoking procedure.

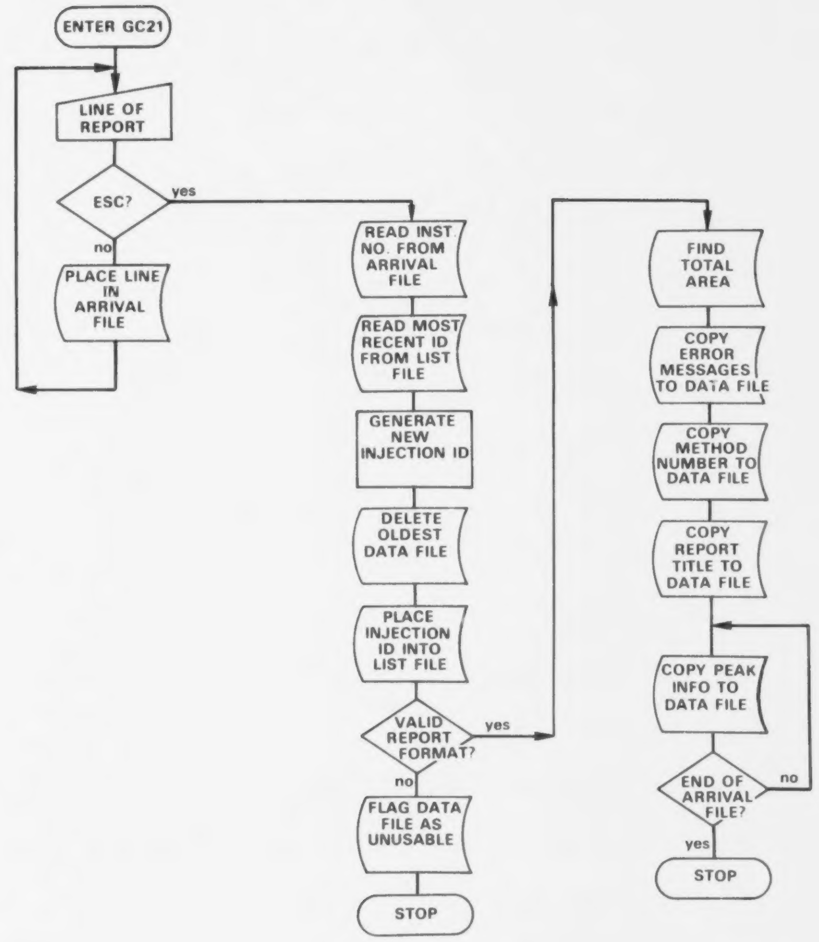

ENTER GC21
LINE OF REPORT
ESC?
yes
no
PLACE LINE IN ARRIVAL FILE
READ INST. NO. FROM ARRIVAL FILE
READ MOST RECENT ID FROM LIST FILE
GENERATE NEW INJECTION ID
DELETE OLDEST DATA FILE
PLACE INJECTION ID INTO LIST FILE
VALID REPORT FORMAT?
yes
no
FLAG DATA FILE AS UNUSABLE
STOP
FIND TOTAL AREA
COPY ERROR MESSAGES TO DATA FILE
COPY METHOD NUMBER TO DATA FILE
COPY REPORT TITLE TO DATA FILE
COPY PEAK INFO TO DATA FILE
END OF ARRIVAL FILE?
no
yes
STOP

Figure 19. Flowchart of Program GC21.

TABLE 17. SYMBOL DEFINITIONS FOR PROGRAM GC21

A	the total area of all peaks in the report
A$	a line of the report
A2$	a holding variable for the value of A$
B	the retention time of a compound
B$	the instrument number
C	the area of a single peak
C$	the name of the ID list file
D$	the name of the data file created
D2$	the name of a previously created data file
E$	the method number
F$	the report title (or the word NONE)
G$	the identifier of a compound
H$	the peak type
I	the control variable for several loops
T1	the record number of the last record used in the data file
W	the number of lines that have been input
Y	the sequence number

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  1
                       PROGRAM LISTING FOR GC21

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0010 REM    +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM    +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM              +
0030 REM    +   PROGRAM GC21, MICROCOMPUTER INTERFACE             +
0040 REM    +   BY:  J. KOPKE (SWORCC), JANUARY 18, 1979          +
0045 REM    +   MOST RECENT REVISION:  MAY 1, 1979                +
0050 REM    +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 DIM A$[72],A2$[72],B$[2],C$[8],D$[10],E$[10],F$[30],G$[8],H$[2]
0090 REM    -------------------------------------------------------
0100 REM            INPUT LINES FROM MICRO; STORE IN ARRIVAL FILE
0110 ON ERR THEN GOTO 0150
0120 OPEN FILE[1,1],"GC00000000"
0130 ON ERR THEN STOP
0140 GOTO 0180
0150 ON ERR THEN STOP
0160 DELAY =1
0170 GOTO 0110
0180 LET W=0
0190 ON ESC THEN GOTO 0520
0200 ON ERR THEN GOTO 0220
0210 INPUT "?",A$
0220 ON ERR THEN STOP
0230 ON ESC THEN STOP
0240 IF A$="" THEN GOTO 0190
0250 IF W=0 THEN GOTO 0480
0260 IF A$[1,6]<>"  GC  " THEN GOTO 0480
0270 REM    -----------------------------------
0280 REM      HANDLE FIRST OF TWO MERGED REPORTS
0285 LET A2$=A$
0290 CLOSE FILE[1]
0300 GOSUB 1620
0305 ON ERR THEN GOTO 0310
0308 DELETE D$
0310 ON ERR THEN GOTO 0350
0320 OPEN FILE[3,0],D$,31
0330 ON ERR THEN STOP
0340 GOTO 0380
0350 ON ERR THEN STOP
0360 DELAY =1
0370 GOTO 0310
0380 WRITE FILE[3,1],2,D$,0

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  2
                       PROGRAM LISTING FOR GC21

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0390 CLOSE FILE[3]
0400 ON ERR THEN GOTO 0440
0410 OPEN FILE[1,1],"GC00000000"
0420 ON ERR THEN STOP
0430 GOTO 0470
0440 ON ERR THEN STOP
0450 DELAY =1
0460 GOTO 0400
0470 LET W=0
0475 LET A$=A2$
0480 LET W=W+1
0490 PRINT FILE[1],A$
0500 GOTO 0190
0510 REM    -------------------------------------------------------
0520 REM            COMPACT ARRIVAL FILE INTO DATA FILE
0530 ON ESC THEN STOP
0540 CLOSE FILE[1]
0550 GOSUB 1620
0560 REM    --------------------------------------
0570 REM      CHECK FOR VALID REPORT FORMAT
0580 ON ERR THEN GOTO 0620
0590 OPEN FILE[1,3],"GC00000000"
0600 ON ERR THEN STOP
0610 GOTO 0650
0620 ON ERR THEN STOP
0630 DELAY =1
0640 GOTO 0580
0650 LREAD FILE[1],A$
0660 IF EOF(1)<>1 THEN GOTO 0770
0665 ON ERR THEN GOTO 0670
0668 DELETE D$
0670 ON ERR THEN GOTO 0710
0680 OPEN FILE[3,0],D$,31
0690 ON ERR THEN STOP
0700 GOTO 0740
0710 ON ERR THEN STOP
0720 DELAY =1
0730 GOTO 0670
0740 WRITE FILE[3,1],3,D$,0
0750 CLOSE FILE[3]
0755 CLOSE FILE[1]
0760 STOP

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  3
                        PROGRAM LISTING FOR GC21

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0770 IF A$<>"  PEAK    NAME   TYPE        COMP     RETN     CORR     A
*    REA    FACTOR" THEN GOTO 0650
0780 REM  ------------------------------------------
0790 REM     FIND TOTAL AREA OF ALL PEAKS
0800 LREAD FILE[1],A$
0810 IF A$[1,12]<>"  TOTAL AREA" THEN GOTO 0800
0820 LET A=VAL(A$[13,23])
0830 CLOSE FILE[1]
0835 ON ERR THEN GOTO 0840
0838 DELETE D$
0840 ON ERR THEN GOTO 0880
0850 OPEN FILE[3,0],D$,31
0860 ON ERR THEN STOP
0870 GOTO 0910
0880 ON ERR THEN STOP
0890 DELAY =1
0900 GOTO 0840
0910 WRITE FILE[3,1],1,D$,0
0920 LET T1=1
0930 REM  ------------------------------------------
0940 REM     SCAN REPORT FOR ERROR MESSAGES
0950 ON ERR THEN GOTO 0990
0960 OPEN FILE[1,3],"GC00000000"
0970 ON ERR THEN STOP
0980 GOTO 1020
0990 ON ERR THEN STOP
1000 DELAY =1
1010 GOTO 0950
1020 LREAD FILE[1],A$
1030 IF EOF(1) THEN GOTO 1080
1040 IF A$[1,7]<>"MESSAGE" THEN GOTO 1020
1050 WRITE FILE[3,T1+1],A$
1060 LET T1=T1+1
1070 GOTO 1020
1080 CLOSE FILE[1]
1090 REM  ------------------------------------------
1100 REM     FIND VARIAN METHOD NUMBER
1110 ON ERR THEN GOTO 1150
1120 OPEN FILE[1,3],"GC00000000"
1130 ON ERR THEN STOP
1140 GOTO 1180
1150 ON ERR THEN STOP

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                     PAGE  4
                        PROGRAM LISTING FOR GC21

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1160 DELAY =1
1170 GOTO 1110
1180 LREAD FILE[1],A$
1190 IF A$[1,6]<>"  INST" THEN GOTO 1180
1200 IF LEN(A$)<=39 THEN LET E$=A$[31,LEN(A$)]
1205 IF LEN(A$)>39 THEN LET E$=A$[31,39]
1210 WRITE FILE[3,T1+1],E$
1220 LET T1=T1+1
1230 REM  ------------------------------------------
1240 REM     FIND REPORT TITLE, IF ANY
1250 LREAD FILE[1],A$
1260 IF A$[1,7]="MESSAGE" THEN GOTO 1250
1270 IF A$[1,6]="  PEAK" THEN GOTO 1300
1280 LET F$=A$[17,LEN(A$)]
1285 IF F$="                                " THEN GOTO 1300
1290 GOTO 1310
1300 LET F$="NONE"
1310 IF F$[LEN(F$)]<>" " THEN GOTO 1319
1311 LET F$=F$[1,LEN(F$)-1]
1312 GOTO 1310
1319 WRITE FILE[3,T1+1],F$
1320 LET T1=T1+1
1330 REM  ------------------------------------------
1340 REM     IGNORE LINES NOT DESCRIBING PEAKS
1350 ON ERR THEN STOP
1360 LREAD FILE[1],A$
1370 IF EOF(1)<>1 THEN GOTO 1410
1380 CLOSE FILE[1]
1390 CLOSE FILE[3]
1400 STOP
1410 ON ERR THEN GOTO 1350
1420 LET D=VAL(A$[1,6])
1430 ON ERR THEN STOP
1500 REM  ------------------------------------------
1510 REM     COPY IDENTIFIER, TYPE, RETENTION TIME, AND AREA
1520 LET G$=A$[9,16]
1521 IF G$[LEN(G$)]<>" " THEN GOTO 1530
1522 LET G$=G$[1,LEN(G$)-1]
1523 GOTO 1521
1530 IF G$="  UNEXP" THEN LET G$="XXXXXXXX"
1535 LET H$=A$[19,20]
1540 LET B=VAL(A$[34,41])

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                         PAGE  5
                        PROGRAM LISTING FOR GC21

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1550 LET C=A*VAL(A$[51,62])/100
1560 WRITE FILE[3,T1+1],G$,H$,B,C,0,0
1570 LET T1=T1+1
1580 GOTO 1350
1590 REM
1600 REM
1610 REM    +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
1620 REM          SUBROUTINE TO CREATE DATA FILE NAME AND
1630 REM               PUSH IT INTO THE LIST FILE GC0000**
1640 REM    --------------------------------------
1650 REM      FIND INSTRUMENT NUMBER
1660 ON ERR THEN GOTO 1700
1670 OPEN FILE[1,3],"GC00000000"
1680 ON ERR THEN STOP
1690 GOTO 1730
1700 ON ERR THEN STOP
1710 DELAY =1
1720 GOTO 1660
1730 LREAD FILE[1],A$
1740 IF EOF(1)<>1 THEN GOTO 1750
1741 LET A$="  INST    99"
1750 IF A$[1,6]<>"  INST" THEN GOTO 1730
1760 CLOSE FILE[1]
1770 LET B$=A$[11,12]
1780 REM    --------------------------------------
1790 REM      OPEN ID LIST FILE; FILL IT WITH
1800 REM            DUMMY ID'S IF IT IS NEW
1810 IF B$[1,1]=" " THEN LET B$[1,1]="0"
1820 LET C$="GC0000",B$
1830 ON ERR THEN GOTO 1850
1840 RENAME C$,C$
1850 ON ERR THEN STOP
1860 IF SYS(7)<>-48 THEN GOTO 1890
1870 DELAY =1
1880 GOTO 1830
1890 IF SYS(7)<>-9 THEN GOTO 1990
1900 ON ERR THEN GOTO 1940
1910 OPEN FILE[2,0],C$,11
1920 ON ERR THEN STOP
1930 GOTO 1970
1940 ON ERR THEN STOP
1950 DELAY =1

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S   C-H-R-O-M-A-T-O-G-R-A-P-H-Y   A-U-T-O-M-A-T-I-O-N   S-Y-S-T-E-M
7/20/1979                                                         PAGE  6
                        PROGRAM LISTING FOR GC21

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1960 GOTO 1900
1970 GOTO 2105
1980 ON ERR THEN GOTO 2020
1990 OPEN FILE[2,0],C$,11
2000 ON ERR THEN STOP
2010 GOTO 2050
2020 ON ERR THEN STOP
2030 DELAY =1
2040 GOTO 1980
2050 FOR I=1 TO 100
2060   WRITE FILE[2,I],"GC99999999"
2070 NEXT I
2090 REM    --------------------------------------
2100 REM      DETERMINE DATE OF INJECTION
2105 IF A$[48,51]<>"DATE" THEN GOTO 2130
2110 LET D$="GC",B$[1,2],A$[52,55]
2120 GOTO 2180
2130 LET D$="GC",B$[1,2],"0000"
2140 LET D$[7-LEN(STR$(SYS(2))),6]=STR$(SYS(2))
2150 LET D$[9-LEN(STR$(SYS(1))),8]=STR$(SYS(1))
2160 REM    --------------------------------------
2170 REM      DETERMINE SEQUENCE NUMBER
2180 READ FILE[2,1],D2$
2190 IF D$[1,8]=D2$[1,8] THEN GOTO 2220
2200 LET D$[9,10]="01"
2210 GOTO 2270
2220 LET Y=VAL(D2$[9,10])+1
2225 IF Y=100 THEN LET Y=0
2230 LET D$[9,10]="00"
2240 LET D$[11-LEN(STR$(Y)),10]=STR$(Y)
2250 REM    --------------------------------------
2260 REM      DELETE OLDEST DATA FILE
2270 READ FILE[2,100],D2$
2280 ON ERR THEN GOTO 2300
2290 DELETE D2$
2300 ON ERR THEN STOP
2310 REM    --------------------------------------
2320 REM      PUSH DATA FILE NAME INTO LIST FILE
2330 FOR I=99 TO 1 STEP -1
2340   READ FILE[2,I],D2$
2350   WRITE FILE[2,I+1],D2$
2360 NEXT I

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  7
                       PROGRAM LISTING FOR GC21

1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
2370 WRITE FILE[2,1],D$
2380 CLOSE FILE[2]
2390 RFTURN












































1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                      PAGE  8
                        SYMBOL TABLE FOR GC21

SYMROL   REFERENCES
------  ---------------------------------------------------------------
 0110   0170
 0150   0110
 0180   0140
 0190   0240  0500
 0220   0200
 0310   0305  0370
 0350   0310
 0380   0340
 0400   0460
 0440   0400
 0470   0430
 0480   0250  0260
 0520   0190
 0580   0640
 0620   0580
 0650   0610  0770
 0670   0665  0730
 0710   0670
 0740   0700
 0770   0660
 0800   0810
 0840   0835  0900
 0880   0840
 0910   0870
 0950   1010
 0990   0950
 1020   0980  1040  1070
 1080   1030
 1110   1170
 1150   1110
 1180   1140  1190
 1250   1260
 1300   1270  1285
 1310   1290  1312
 1319   1310
 1350   1410  1580
 1410   1370
 1521   1523
 1530   1521
 1620   0300  0550
 1660   1720
 1700   1660
 1730   1690  1750
 1750   1740
 1830   1880
```

```
G-A-S  C-H-R-O-M-A-T-O-G-R-A-P-H-Y  A-U-T-O-M-A-T-I-O-N  S-Y-S-T-E-M
7/20/1979                                                        PAGE  9
                           SYMBOL TABLE FOR GC21

SYMBOL   REFERENCES
------ ---------------------------------------------------------------
 1850  1830
 1890  1860
 1900  1960
 1940  1900
 1970  1930
 1980  2040
 1990  1890
 2020  1980
 2050  2010
 2105  1970
 2130  2105
 2180  2120
 2220  2190
 2270  2210
 2300  2280
 A     0820  1550
 A$    0080  0210  0240  0260  0285  0475  0490  0650  0770  0800
       0810  0820  1020  1040  1050  1180  1190  1200  1205  1250
       1260  1270  1280  1360  1420  1520  1535  1540  1550  1730
       1741  1750  1770  2105  2110
 A2$   0080  0285  0475
 B     1540  1560
 B$    0080  1770  1810  1820  2110  2130
 C     1550  1560
 C$    0080  1820  1840  1910  1990
 D     1420
 D$    0080  0308  0320  0380  0668  0680  0740  0838  0850  0910
       2110  2130  2140  2150  2190  2200  2230  2240  2370
 D2$   2180  2190  2220  2270  2290  2340  2350
 E$    0080  1200  1205  1210
 F$    0080  1280  1285  1300  1310  1311  1319
 FL#1  0120  0290  0410  0490  0540  0590  0650  0755  0800  0830
       0960  1020  1080  1120  1180  1250  1360  1380  1670  1730
       1760
 FL#2  1910  1990  2060  2180  2270  2340  2350  2370  2380
 FL#3  0320  0380  0390  0680  0740  0750  0850  0910  1050  1210
       1319  1390  1560
 G$    0080  1520  1521  1522  1530  1560
 H$    0080  1535  1560
 I     2050  2060  2070  2330  2340  2350  2360
 T1    0920  1050  1060  1210  1220  1319  1320  1560  1570
 W     0180  0250  0470  0480
 Y     2220  2225  2240
```

SECTION 24

FILE STRUCTURES

The following tables detail the structure of the files used in the GCAS.

TABLE 18. STRUCTURE OF THE SAMPLE FILE CONTROL RUN RESULTS FILE

Name of file: PPPPPPPA.RR where PPPPPPP = parameter/method code
A = a letter of the alphabet

File Number: 0

Contents

This is a sequential file consisting of eighty-byte strings. The format of the strings and their order are defined in the Sample File Control Foreground BASIC Functional Design.

TABLE 19. STRUCTURE OF THE ARRIVAL FILE

Name of file: GC00000000

File Number: 1

Contents

This is a sequential file. The report is placed in this file one line at a time as it is received from the microcomputer. Each line is a string of at most 70 characters.

TABLE 20. STRUCTURE OF THE ID LIST FILE

Name of file: GC0000II where II = instrument number

File Number: 2

Record Length: 11 bytes

Record	Contents
1	most recent D$
2	second most recent D$
3	third most recent D$
.	.
.	.
.	.
100	hundredth most recent D$

where D$ = the name of a data file

TABLE 21. STRUCTURE OF THE INJECTION DATA FILE

Name of file:	GCIIMMDDSS	where II = instrument number MM = month DD = day SS = sequence number
File Number:	3	
Record Length:	31 bytes	

Record	Contents	
1	J, D$, J2	where J = data file useability flag 1. good data 2. no TOTAL AREA 3. wrong format D$ = name of the data file J2 = status flag 1. has been processed 2. never processed
2	VO$	where VO$ = MESSAGE (if any)
n+2	E$	where E$ = method number
n+3	F$	report title
n+4	G$,H$,B,C,L,L2	where G$ = identifier H$ = peak type B = absolute retention time C = peak area L = calculated concentration L2 = calculated relative retention time
n+5	G$,H$,B,C,L,L2	
.	.	
.	.	
.	.	where n = number of error messages

TABLE 22. STRUCTURE OF THE METHOD FILE

Name of file: GCMMMM where MMMM = method number

File Number: 4

Record Length: 200 bytes

Record	Contents	
1	T$,U$,N1,N2,N$	where T$ = name of method file U$ = name of user N1 = type of method 1. internal standards 2. purge and trap 3. liquid/liquid 4. direct aqueous N2 = type of retention time 1. relative 2. capacity ratio N$ = identifier for relative retention time reference compound, or capacity ratio dead volume time as a string
3i-1	V$,V1$,V2$,V3$,V4$,V5$,V6$	where V$ = identifier V1$ = first compound name V2$ = first CAS number V3$ = second compound name V4$ = second CAS number V5$ = third compound name V6$ = third CAS number
3i	D4$,I$,K,R1,R2,R3,J3	where D4$ = date of calibration I$ = superstring of injection IDs of standards K = type of fit 1. linear regression 2. quadratic regression 3. linear interpolation 4. linear regression forced through origin R1 = constant term of equation R2 = linear term of equation R3 = quadratic term of equation J3 = fitting error

TABLE 22. (Continued)

Record	Contents
3i+1	G(i,1),G(i,2),G(i,3),....,G(i,30) where G(i,odd) = concentration G(i,even) = area
3i-1	V\$,V1\$,V2\$,V3\$,V4\$,V5\$,V6\$
3i	D4\$,I\$,K,R1,R2,R3,J3
3i+1	G(i,1),G(i,2),G(i,3),....,G(i,30)
.	.
.	.
.	.
.	.
.	.
.	.
.	.
.	.
.	.

where i = counter for identifiers

TABLE 23. STRUCTURE OF THE TEMPORARY FORMATTED OUTPUT FILE

Name of file: GCOMMMM where MMMM = method number

File Number: 5

Contents

This is a sequential file. The formatted output report is placed into this file line by line as it is generated. Each line is a string of at most 132 characters.

TABLE 24. STRUCTURE OF THE CONCENTRATION PATTERN FILE

Name of file: GGMMMMOSS where MMMM = method number
SS = sequence number matching a letter of the alphabet

File Number: 7

Record Length: 4 bytes

Record	Contents
1	A5 for first identifier
2	A5 for second identifier
3	A5 for third identifier
.	.
.	.
.	.
.	.

where A5 = the known concentration